



NESCC HPC Group A End User Training
Dan Schornak (CSC)
Shawn Hoopes (Adaptive Computing)

TRAINING AGENDA – Group A

- 0800-0810 Training Process
- Introduce instructors
 - General information
 - Define training roles and responsibilities
 - Review training agenda
- 0810-0815 Training Objectives
- Review the objectives of the NESCC HPC Environment overview
- 0815-0845 Introduction to NESCC HPC Design/Architecture and Environment
- Describe the overall architecture major components, functions, and features
- 0845-0900 Available On-line Documentation
- 0900-0915 **BREAK**

TRAINING AGENDA – Group A

- 0915-0945 Introduction to User Environment, Policies, Quotas,
and Environmental Variables
- 0945-1045 Introduction to Programming Environment
- Introduce tools – shells, applications, compilers, and libraries
- 1045-1145 Introduction to NESCC Storage and Data Management
- 1145-1245 **LUNCH BREAK**
- 1245-1415 Introduction to Job Scheduling using Moab (Adaptive Computing)
- Efficient job submission techniques
 - Installed NESCC version compared to other NOAA installations
 - Moab/Torque end-user commands and tools
- 1415-1500 Questions/Answers
- 1500 Session Wrap up

Need Help? – Where to go...

Zeus User Support and Problem Reporting (Help Desk for NESCC)
rdhpcs.zeus.help@noaa.gov

HPSS User Support and Problem Reporting (Help Desk for NESCC)
rdhpcs.hpss.help@noaa.gov

NESCC FAQ and Documentation Wiki Site – “How to...”
https://nescdocs.rdhpcs.noaa.gov/wiki/index.php/Main_Page

End User Experience

EMC Model Transition Team (Provides updates for porting to TDS and Zeus)
<http://www.emc.ncep.noaa.gov/mtt>

NESCC Factoid...

“Documentation will continue to be updated on NescDocs.”

Need Help? – Where to go...

[NESCC Documentation Wiki Site – “How to...”](https://nescdocs.rdhpcs.noaa.gov/wiki/index.php/Main_Page)

https://nescdocs.rdhpcs.noaa.gov/wiki/index.php/Main_Page

The screenshot shows a Windows Internet Explorer browser window displaying the 'Main Page' of the NESCC Documentation Wiki. The address bar shows the URL https://nescdocs.rdhpcs.noaa.gov/wiki/index.php/Main_Page. The page content includes a navigation sidebar on the left with links like 'Main page', 'Community portal', and 'Recent changes'. The main content area features a 'Main Page' heading, a notice about the Zeus RDHPCS Documentation System, and several categorized lists of links for navigation, getting started, and other information.

Main Page

The Zeus RDHPCS Documentation System is online

Below is information regarding the use of Jet. The original version of this document lives at <https://nescdocs.rdhpcs.noaa.gov>. If you are not at that site, please go there for the latest, up to date information. If you have any questions or comments regarding the material, please email the Help system.

NOTICE — The configuration of Zeus is moving along quickly. We are still learning the best way to setup the system. Expect this information and the configuration to change daily until roughly January 15th, 2012.

- Overview
 - About NESCC
 - Policy and Procedures
 - Architecture Overview
 - System Configuration
- Getting Started
 - Getting an Account
 - Logging in to Zeus
 - Transferring Data
 - Requesting Help
 - Getting Information About Your Account
- Getting Things Done
 - Using Modules
 - Using the Compilers
 - Using MPI
 - Running and Monitoring Jobs
 - Using the Workflow Manager
 - Debugging Codes
 - Profiling Codes
 - Starting Recurring Processes with Cron
- Other Information
 - Why is My Job Not Running
 - Notes on Building and Running Common Applications
 - User Manuals, Reference Guides, and Links to Resources
 - Previously Asked Questions

Need Help? – Where to go...

End User Experience

EMC Model Transition Team (Provides updates for porting to TDS and Zeus)

<http://www.emc.ncep.noaa.gov/mtt>

The screenshot shows a web browser window displaying the National Weather Service Environmental Modeling Center website. The browser's address bar shows the URL <http://www.emc.ncep.noaa.gov/mtt/zeus.php>. The website header includes the NOAA logo and the text "National Weather Service Environmental Modeling Center". Navigation links for "Home", "News", and "Organization" are visible. The main content area is titled "MISSION / VISION About EMC" and "EMC > MTT >". A breadcrumb trail shows "Home > Meeting Minutes > GAEA > ZEUS > Help". The "Model Transition Team" section contains two columns: "TRAINING AND DOCUMENTATION MATERIALS:" and "NEWS AND UPDATES:". The "TRAINING AND DOCUMENTATION MATERIALS:" section lists items such as "Compiling and running on Zeus", "Interim documentation regarding Zeus/TDS", "NESCC login node usage policy and system limits", "Architecture Overview", "System Configuration", and "User Manuals, Reference Guides, and Links to Resources". The "NEWS AND UPDATES:" section features a dated entry: "01/24/12 (from UN IBM notes) TDS benchmark tests are finished. The deadline for general user access to Zeus is 01/30; all users with Vapor accounts will be automatically transfer to Zeus in Feb & a list of EMC users who should apply for Vapor/Zeus accounts was compiled by EMC (only 27 tokens left & CSC will send 25 more), Vapor tokens (& pins) will automatically work on Zeus. A user survey on when to hold Zeus training is going on today; a Zeus user GTM/telecon is scheduled for 01/25 (1100) in 209 & 802. Vapor is scheduled to be shut down ~May. TDS/Zeus tickets should be sent to rdhpcs.zeus.help@noaa.gov. Data transfer between CCS/Zeus is being worked by NCO network group." Below this, there is a section for "Zeus Group A End User Training - December 15th" which lists training presentations: "NOAA Training Slides (Group A)" and "Moab Training Presentation (Group A)". A "Logging into Zeus" section describes a method by Daryl Kleist, noting that after entering a pin+RSA, it may ask for a certificate passphrase. A terminal-style error message is displayed: "No proxy certificate found, generating. Expired or nonexistent proxy certificate. Please enter your certificate passphrase: Error: Couldn't find valid credentials to generate a proxy. Use -debug for further information. grid-proxy-init failed". A vertical sidebar on the right edge of the page reads "National Weather Service - Since 1870".

TRAINING OBJECTIVES (Group A)

<i>What it is...</i>	<i>What it isn't...</i>
Introduction to NESCC HPC Environment	System Administrator-level Training
User Environment Overview	Unix scripting Overview
Programming Environment Overview	Application/System Tuning Overview
Introduction to Moab Workload Manager/Torque Resource Manager	Moab Administrator-level Training

Disclaimer: As Zeus moves through its acceptance period, some training content may become obsolete. For the latest guidance on how to use these NESCC HPC resources, please visit the following site regularly:

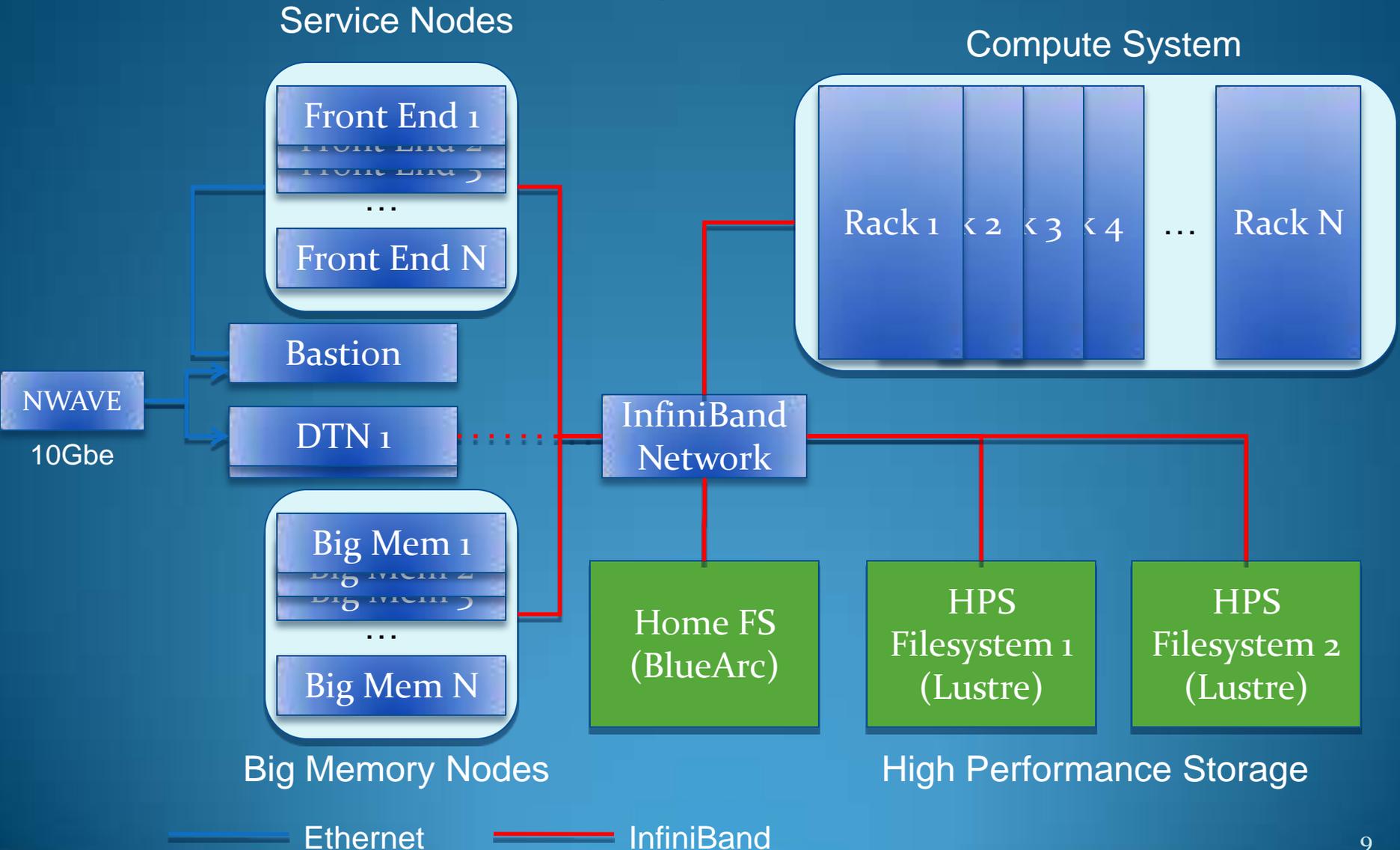
<https://nescdocs.rdhpcs.noaa.gov>

NESCC HPC Design/Architecture and Environment

Type	Purpose
Bastion	All login sessions are routed through these hosts. They provide additional security to protect NOAA assets.
Service Nodes	Where initial login sessions are created. They are for general interactive use for operations such as editing and compiling code, managing files, initiating actions on external network including data transfer and accessing software repository.
Data Transfer Nodes (DTN)	Provide high speed Inbound and outbound data transfers. - FOR EXTERNALLY INITIATED TRANSFERS -
Compute System	Major compute resources for parallel jobs. Accessible through the batch system.
Big Memory Nodes	Large memory set for applications that require more memory than a single compute node. Accessible through the batch system.
High Performance Storage	High speed filesystems
Home Filesystem	Storage system optimized for editing and compiling code.

NESCC HPC Design/Architecture and Environment

Zeus/Herc System Architecture



NESCC HPC Design/Architecture and Environment

Zeus System Configuration

Subsystem	Size
Service Nodes	8 (48 GB/node)
Big Memory Nodes	6 (96 GB/node)
Compute Nodes	2304
Compute Cores	27648
Total Flops	383 TF
Total Data Transfer Nodes	2+
HPS Capacity	5.6 PB
HPS Performance	> 70 GB/s

- There will be several DTN types depending on location of originating connection. Policy is being finalized by NOAA management.

General System Information

Node Type	Total Cores	Core Speed	Memory	Local Storage
Service	12	3.46GHz	48 GB	Yes
Compute	12	3.46GHz	24 GB	No
Big Memory	12	3.46GHz	96 GB	No

Notes:

- There are no CRON Nodes. CRON Services will be provided on Zeus through a NOAA developed system that unifies the crontab across all login nodes.

NESCC HPC Design/Architecture and Environment

Test and Development System (TDS)

Test LSC System Components (Herc)
HPC System: SGI Altix ICE 8400 EX
Filesystem: Lustre

Login Node: tfe1

TDS (a.k.a Herc) - SGI ICE

- 48 nodes, 3.46 GHz Intel Westmere
- 12 cores per node
- 2GB per core (24GB per node)
- QDR dual-rail InfiniBand
- Lustre

The fast parallel filesystem mount points are /tds_scratch1 and /tds_scratch2. You can create directories for your use under the *users* directory.

~source: https://nescdocs.rdhpcs.noaa.gov/wiki/index.php/Access_and_Use_of_TDS

NESCC Factoid...

“TDS is for testing new software components, debugging system problems, and testing applications as necessary. Users will only have access when granted to solve specific problems. This is not a generally accessible resource.”

NESCC HPC Design/Architecture and Environment

Zeus Production System

Production LSC System Components (Zeus)

SGI Altix ICE 8400 EX

Filesystem: Lustre

Login Nodes: fe1

fe2

fe3

fe4

fe5

fe6

fe7

fe8

SGI ICE – Zeus Compute Nodes

2304 IP-105 blades

4608 CPUs, X5690 e.46GHz 6-Core

24 GB DDR3 1333MHz 2 cores per node

4GB per core (48GB per node)

QDR dual-rail InfiniBand

Lustre

The fast parallel filesystem mount points are /scratch₁ and /scratch₂.
Users are assigned projects, and those projects have preexisting storage in directories in /scratch₁ and /scratch₂.

NESCC HPC Design/Architecture and Environment

Data Storage

Production LSC System Components (Zeus)

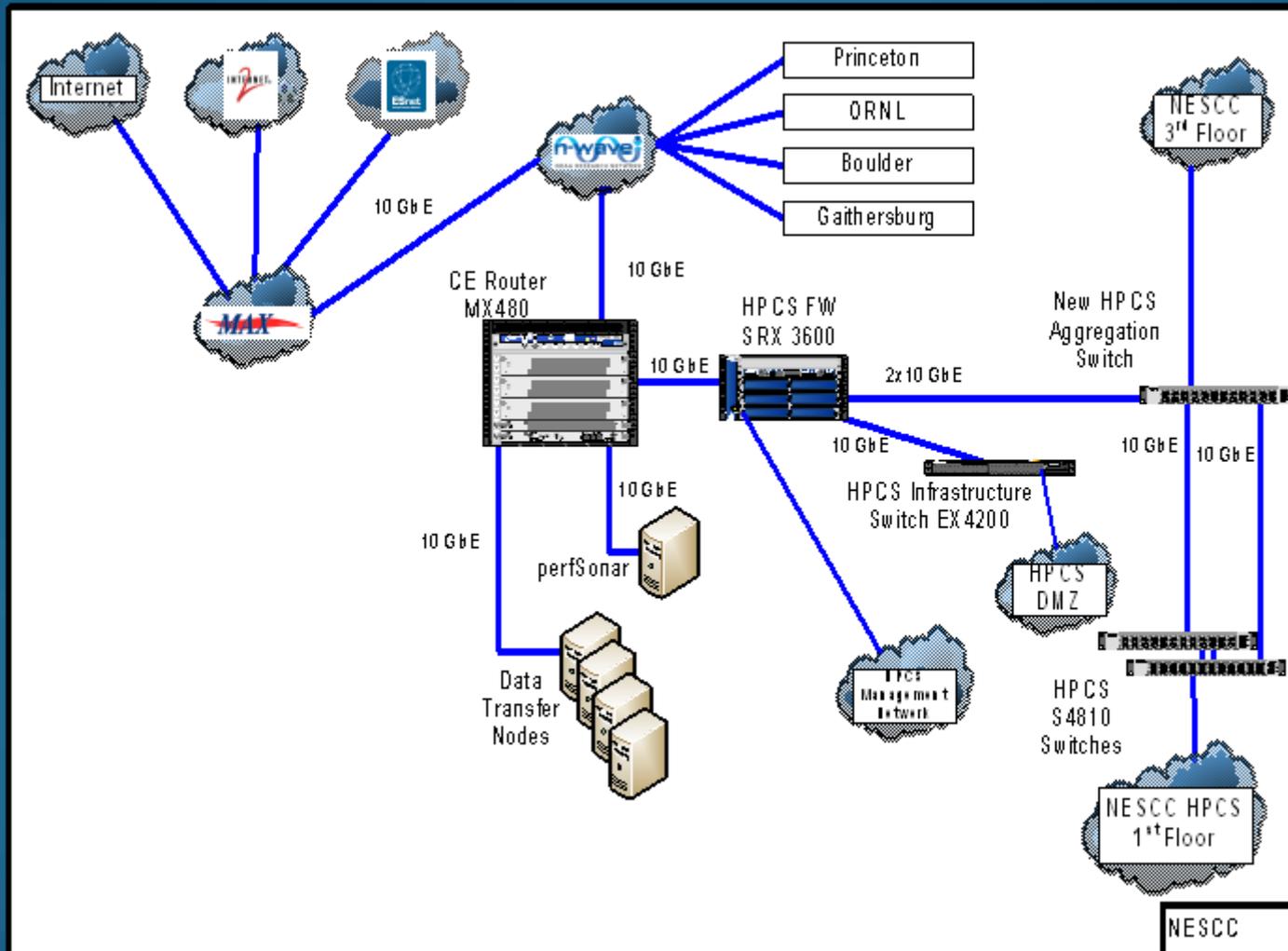
SGI Altix ICE 8400 EX

Filesystem: Lustre

HPSS production system has a 1 PB disk cache
Oracle SL8500 Modular Library with 32 T10Kc drives.
The library has slots for 10000 tapes (50 PB) max capacity, but only
7500 tapes are in the silo at this time (37.5PB).

NESCC HPC Design/Architecture and Environment

Wide Area Network



Available Online Documentation – Good to Know

NESCC Documentation Wikisite:	https://nescdocs.rdhpcs.noaa.gov/
NESCC TDS Wikisite:	https://nescdocs.rdhpcs.noaa.gov/wiki/index.php/Access and Use of TDS
EMC Model Transition Team Website:	http://www.emc.ncep.noaa.gov/mtt

Compilers

- Intel Fortran Users' Guide:
<http://software.intel.com/sites/products/documentation/hpc/composerxe/en-us/2011Update/fortran/lin/index.htm>
- Intel C/C++ Users' Guide:
<http://software.intel.com/sites/products/documentation/hpc/composerxe/en-us/2011Update/cpp/lin/index.htm>
- Intel Math Kernel Library Users' Guide:
http://software.intel.com/sites/products/documentation/hpc/composerxe/en-us/2011Update/mklxe/mkl_userguide_lnx/index.htm
- Intel Compiler Optimization Guide:
http://software.intel.com/sites/products/collateral/hpc/compilers/compiler_grq12.pdf
- PGI Compiler User's Guide for Parallel Fortran, C and C++: <http://www.pgroup.com/doc/pgiug.pdf>
- PGI Compiler Reference Manual for Parallel Fortran, C and C++: <http://www.pgroup.com/doc/pgiref.pdf>
- PGI Fortran Reference: <http://www.pgroup.com/doc/pgifortref.pdf>

Available Online Documentation – Good to Know

MPI Libraries

- Message Passing Toolkit (MPT) User's Guide:
http://techpubs.sgi.com/library/tpl/cgi-bin/browse.cgi?coll=linux&db=bks&cmd=toc&pth=/SGI_Developer/MPT_UG

SGI

- Linux® Application Tuning guide for SGI® X86-64 Based Systems:
http://techpubs.sgi.com/library/tpl/cgi-bin/browse.cgi?coll=linux&db=bks&cmd=toc&pth=/SGI_Developer/LX_86_AppTune

IBM Documentation

- HPSS User Guides: http://www.hpss-collaboration.org/user_doc.shtml

Archival Documentation

- HTAR Man Page: http://www.mgleicher.us/GEL/htar/htar_man_page.html
- HTAR User Guide: http://www.mgleicher.us/GEL/htar/htar_user_guide.html
- HSI Commands (Alphabetical List): http://www.mgleicher.us/GEL/hsi/hsi_reference_manual_2/hsi_commands_-_alphabetical.html

Administrative Book – Nice to Know

- SGI® Performance Suite 1.3 Start Here:
http://techpubs.sgi.com/library/tpl/cgi-bin/browse.cgi?coll=linux&db=bks&cmd=toc&pth=/SGI_Admin/PS_Start_Here

Available Online Documentation – Nice to Know

Administrative Books

- SGI® Performance Suite 1.3 Start Here:

http://techpubs.sgi.com/library/tpl/cgi-bin/browse.cgi?coll=linux&db=bks&cmd=toc&pth=/SGI_Admin/PS_Start_Here

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Introduction to User Environment, Policies, Quotas, and Environmental Variables

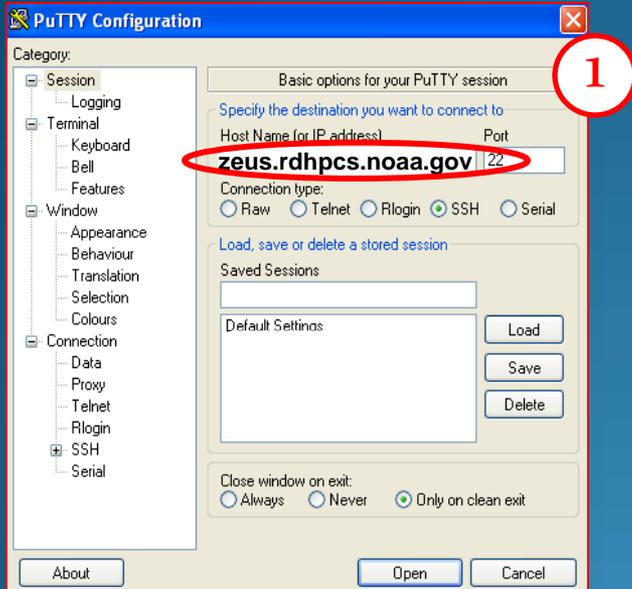
Section Objectives

1. Investigate various login approaches to TDS/Zeus
2. Review and explore the User Environment
3. Learn how to establish an SSH Tunnel
4. Knowing the Limitations – Established Policies and Quotas



LOGGING IN – Getting from here to there

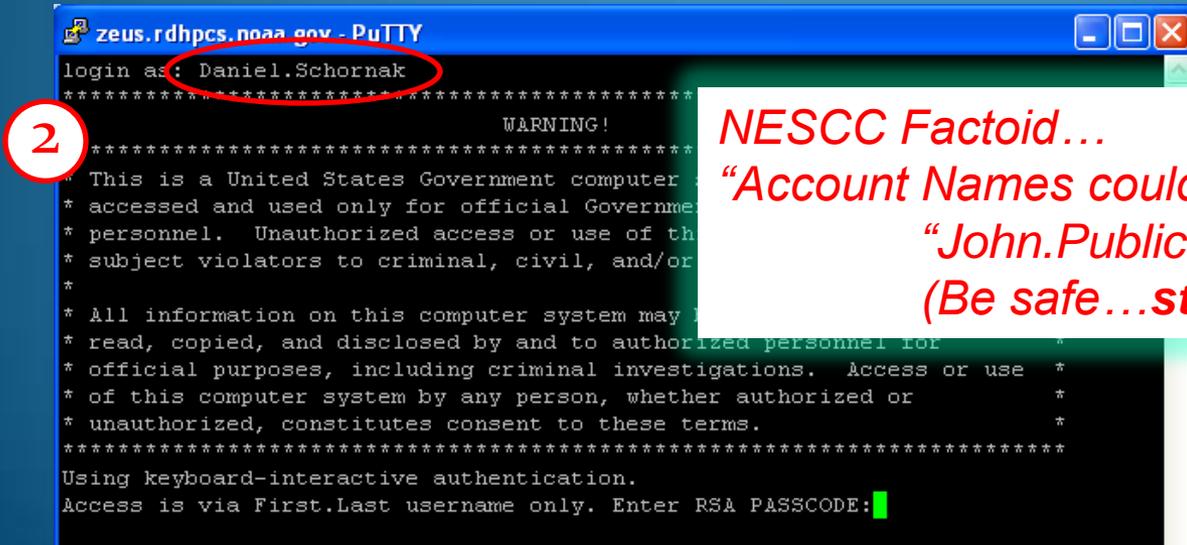
PuTTY Example to TDS



1. Start PuTTY (**Host Name: zeus.rdhpcs.noaa.gov**)
2. Log into zeus
3. Hit ^C within 5 seconds
4. Enter “tfe1”
5. You’re now on the TDS!

If password-less login has not yet been established

1. Enter the default password: Pa\$\$w0rd (that’s zero!)
2. Upon entry, please change your password (*passwd*)



NESSC Factoid...

**“Account Names could be in the form of...
“John.Public” or “John.Q.Public”
(Be safe...stay case sensitive)**

LOGGING IN – Getting from here to there

PuTTY Example to TDS (continued)

3

```
zeus.rdhpcs.noaa.gov - PuTTY
login as: Daniel.Schornak
*****
*
* This is a United States
* accessed and used only by
* personnel. Unauthorized
* subject violators to cri
*
* All information on this
* read, copied, and disclo
* official purposes, inclu
* of this computer system
* unauthorized, constitute
*****
Using keyboard-interactive
Access is via First.Last u
Last login: Fri Nov 11 21:
Welcome to the NOAA RDHPCS
Certificate unavailable, f
CSR not found in LDAP, and
You will now be connected
Hit ^C within 5 seconds to
```

1. Start PuTTY (**Host Name: zeus.rdhpcs.noaa.gov**)
 2. Log into zeus
 3. Hit ^C within 5 seconds
 4. Enter "tfe1"
 5. You're now on the TDS!
- If password-less login has not yet to be established
1. Enter the default password: Pa\$\$w0rd (that's zero!)
 2. Upon entry, please change your password (passwd)

4

```
zeus.rdhpcs.noaa.gov - PuTTY
*****
Using keyboard-interactive authentication.
Access is via First.Last username only. Enter RSA PASSCODE
Last login: Tue Nov 15 00:49:33 2011 from 206.173.46.196.
Welcome to the NOAA RDHPCS.
Certificate unavailable, falling back to token access.
CSR not found in LDAP, and problems uploading CSR. Will try again on next login.
You will now be connected to OneNOAA RDHPCS: Zeus system
Hit ^C within 5 seconds to select another host.
Menu:
=====
Select a host. Enter the hostname, or a unique portion of a hostname:
Hostname      IP Address
bmem1        140.90.206.42
bmem2        140.90.206.43
bmem3        140.90.206.44
bmem4        140.90.206.45
bmem5        140.90.206.46
bmem6        140.90.206.47
bqgs1        140.90.206.48
bqgs2        140.90.206.49
dtn1         140.90.206.57
dtn2         140.90.206.58
fe1          140.90.206.33
fe2          140.90.206.34
fe3          140.90.206.35
fe4          140.90.206.36
fe5          140.90.206.37
fe6          140.90.206.38
fe7          140.90.206.39
fe8          140.90.206.40
gw1          140.90.206.55
rw2          140.90.206.56
cbqgs1       140.90.206.50
tfe1         140.90.206.41
Enter hostname here: tfe1
```

5

```
Daniel.Schornak@tfe1:~
* 06-Sep-2011
-> Ugraded Moab to Moab 6.1.1 w/o ODBC

* 02-Sep-2011
-> Updated MOAB to use NODECFG Features,
    type 'mdiag -n' or 'mdiag -n -t' for
    node properties.

* 31-Aug-2011
-> Enabled dynamic overclocking (aka Intel TurboBoost)
    and set the scaling governor in Linux to "performance"
-> Added kernel boot options recommended by SGI benchmarking

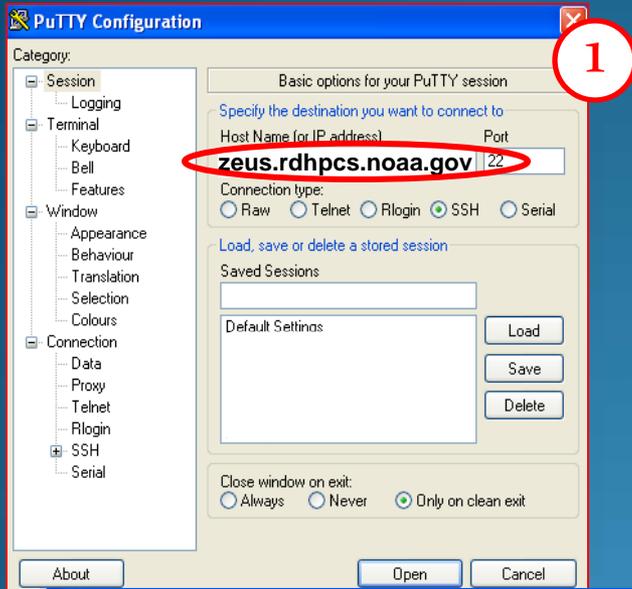
* Before 31-Aug-2011
-> MOAB is now running 6.1
-> Compiler Licenses are restored

type:
module avail
for various Available Modules

[Daniel.Schornak@tfe1 ~]$
```

LOGGING IN – Getting from here to there

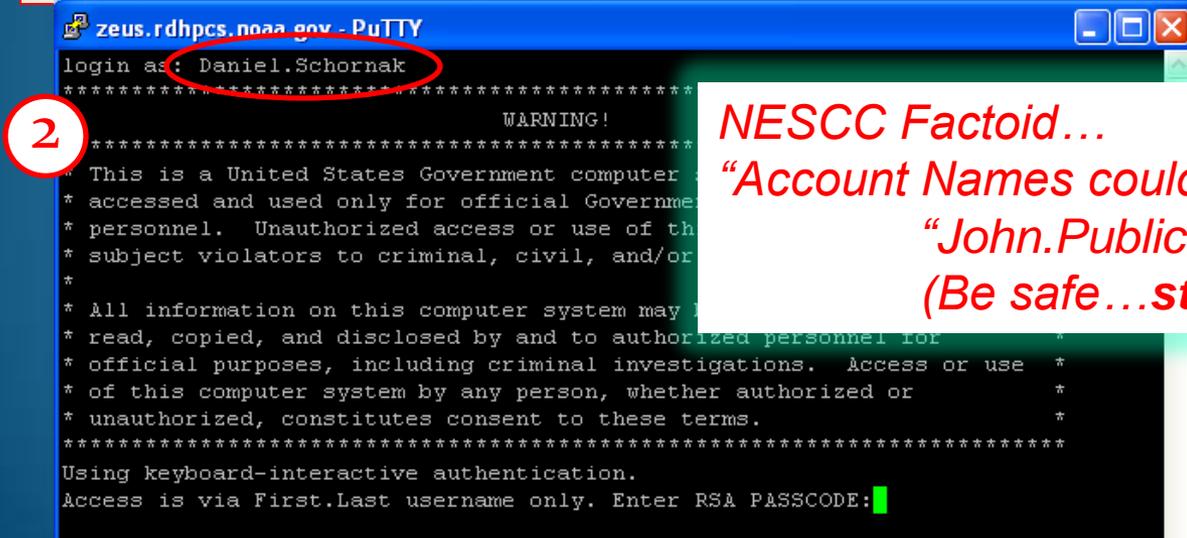
PuTTY Example to Zeus



1. Start PuTTY (**Host Name: zeus.rdhpcs.noaa.gov**)
2. Log into zeus
3. Ignore the ^C prompting - allow 5 seconds to pass
4. You're now on Zeus!

If you require to be on a specific log in node:

1. Enter ^C instead in step 3 above
2. Select your specific login node (fe1 through fe8) – see TDS example



NESSC Factoid...

**“Account Names could be in the form of...
“John.Public” or “John.Q.Public”
(Be safe...stay case sensitive)**

LOGGING IN – Getting from here to there

PuTTY Example to Zeus (continued)

3

zeus.rdhpcs.noaa.gov - PuTTY

```
login as: Daniel.Schornak
*****
*
*                               WARNING!
*                               *****
* This is a United States Governm Daniel.Schornak@fe6:~
* accessed and used only for offi ssh -L21796:localhost:21796
* personnel. Unauthorized access To use the port tunnel for SCP
* subject violators to criminal, -----
*
* All information on this compute scp -P 21796 /local/path/to/file Daniel.Schornak@localhost:/remote/path/to/fi
* read, copied, and disclosed by le
* official purposes, including cr or
* of this computer system by any scp -P 21796 Daniel.Schornak@localhost:/remote/path/to/file /local/path/to/fi
* unauthorized, constitutes conse le
*****
Using keyboard-interactive authen
Access is via First.Last username
Last login: Fri Nov 11 21:33:44 2
Welcome to the NOAA RDHPCS.

Certificate unavailable, falling
CSR not found in LDAP, and proble
You will now be connected to OneM
Hit ^C within 5 seconds to select
```

1. Start PuTTY (**Host Name: zeus.rdhpcs.noaa.gov**)
 2. Log into zeus
 3. Ignore the ^C prompting - allow 5 seconds to pass
 4. You're now on Zeus!
- If you require to be on a specific log in node:
1. Enter ^C instead in step 3 above
 2. Select your specific login node (fe1 through fe8) – see TDS example

4

```
Welcome to the zeus High Performance Computing system

This system is located in Fairmont, WV

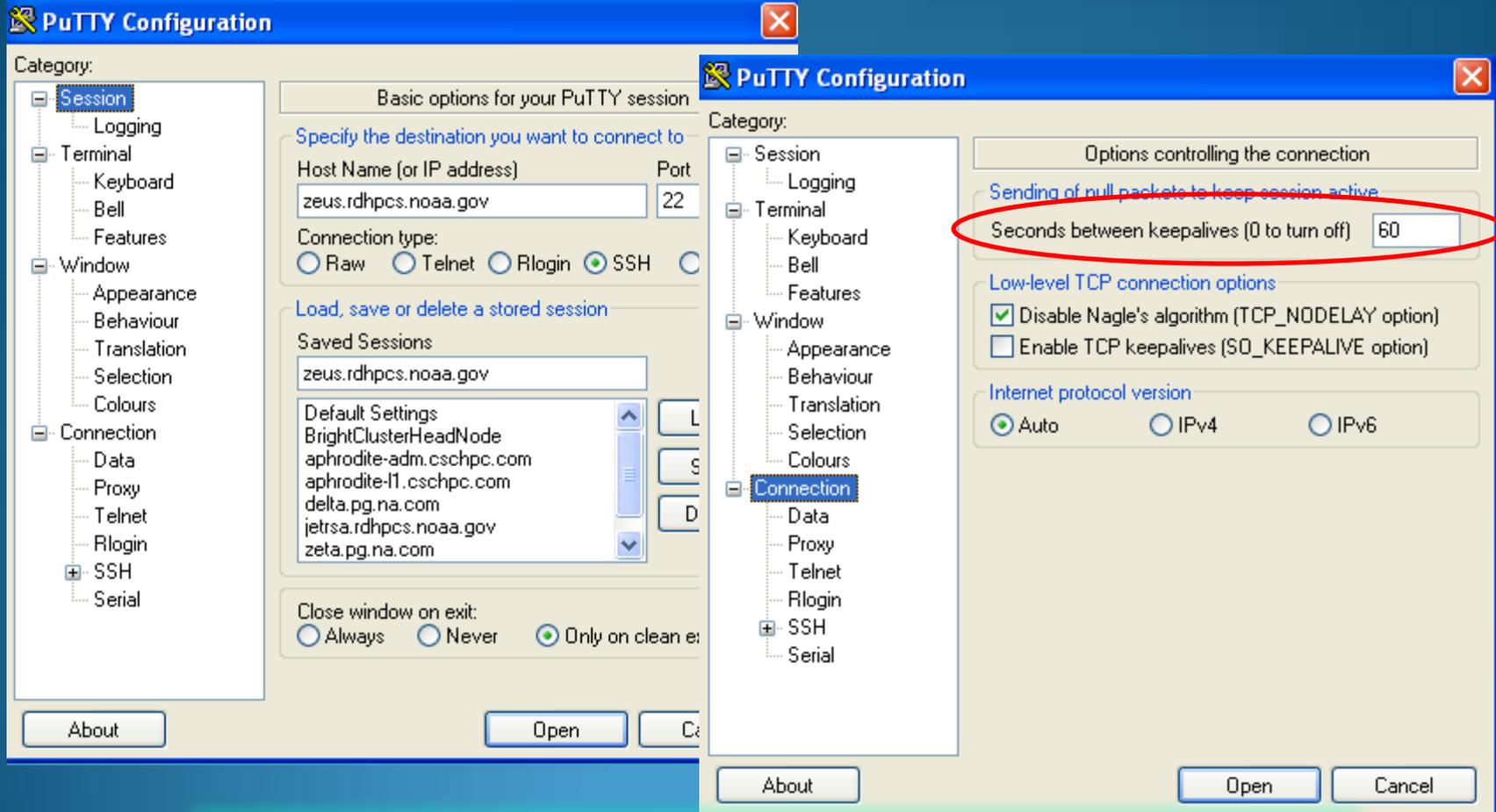
Please Submit Helpdesk Request to:

rdhpcs.zeus.help@noaa.gov
```

```
[Daniel.Schornak@fe6 ~]$
```

Keepalive Packets

PuTTY Example (continued)



NESCC Factoid...

"Avoid connection timeouts by sending 'keepalive' packets"

Getting data from here to there

Data Transfer Approaches

SSH Port Tunnelling - *Outside noaa.gov*

1. PuTTY Example
2. WinSCP Example

Data Transfer Host (*Preferred Approach*) – *Inside noaa.gov*

Unattended Data Transfer – *Inside noaa.gov*

NESCC Factoid...

“DTN support is currently available from NCEP, GFDL, DSRC (Boulder), AOML and NSSL. If your laboratory is not listed and needs DTN access or if a current site cannot access the DTN, send a help request.”

https://nescdocs.rdhpcs.noaa.gov/wiki/index.php/Transferring_Data

TUNNELLING – Getting data from here to there

Linux Example

```
dschorna@aph...-11:~$ ssh Daniel.Schornak@zeus.rdhpcs.noaa.gov
*****
*                               WARNING!                               *
*****
* This is a United States Government computer system. This system is *
* accessed and used only for official Government business by NOAA *
* personnel. Unauthorized access or use of this system may subject *
* subject violators to criminal, civil, and administrative penalties. *
* All information on this computer system is unclassified, but may be *
* read, copied, and disclosed by and to unauthorized personnel. For *
* official purposes, including criminal investigations, the use of *
* of this computer system by any person, without the express written *
* unauthorized, constitutes consent to the release of the information *
*****
Access is via First.Last username only.
```

```
Daniel.Schornak@tfe1:~$ ssh -L21796:localhost:21796 Daniel.Schornak@zeus.rdhpcs.noaa.gov
PLEASE NOTE:
*****
You will need to reconfigure your SSH client to use the tunnel
*and* re-establish a login session to the remote host if you have
if you have never used this port before.

Configure your SSH client to local forward port 21796
to localhost:21796.
For Unix, Linux, and MacOSX users, start ssh like this:

ssh -L21796:localhost:21796 Daniel.Schornak@zeus.rdhpcs.noaa.gov
```

1. Get Your Personal Port Number:
 - a. Log in to Zeus (**zeus.rdhpcs.noaa.gov**)
`ssh Daniel.Schornak@zeus.rdhpcs.noaa.gov`
 - b. Enter password and PIN
 - c. Hit ^C within 5 seconds (*optional*)
 - d. Enter “tfe1” (for TDS) or “fall through” (For Zeus)
 - e. Find port tunnel ID in Welcome Message
 - f. Log out of the session
2. On Linux station, log in with tunnel attributes:
`ssh -L21796:localhost:21796 Daniel.Schornak@zeus.rdhpcs.noaa.gov`
3. Verify tunnel is established in Welcome Message

NESCC Factoid...
“Port number is unique for each user.
Only 1 login session can tunnel

TUNNELLING – Getting data from here to there

Linux Example (continued)

```
dschorna@aphrodite-l1:-  
[dschorna@aphrodite-l1 ~]$ ssh -L21796:localhost:21796 Daniel.Schornak@zeus.rdhpcs.noaa.gov  
*****  
* WARNING!  
*****  
* This is a United States Government  
* accessed and used only for official  
* personnel. Unauthorized access or  
* subject violators to criminal, civil  
*  
* All information on this computer s  
* read, copied, and disclosed by any  
* official purposes, including crim  
* of this computer system by any per  
* unauthorized, constitutes consent  
*****  
Access is via First.Last.username@noaa.gov
```

2

1. ~~Get Your Personal Port Number:~~
 - a. ~~Log in through Zeus (**zeus.rdhpcs.noaa.gov**)~~
`ssh Daniel.Schornak@zeus.rdhpcs.noaa.gov`
 - b. ~~Hit ^C within 5 seconds (Optional)~~
 - c. ~~Enter "tfe1" (for TDS) or "fe1" (For Zeus)~~
 - d. ~~Find port tunnel ID in Welcome Message~~
 - e. ~~Log out of the session~~
2. On Linux station, log in with tunnel attributes:
`ssh -L21796:localhost:21796 Daniel.Schornak@zeus.rdhpcs.noaa.gov`
3. Verify tunnel is established in Welcome Message

3

```
Daniel.Schornak@fe8:-  
Hit ^C within 5 seconds to  
Attention user:  
A port-tunnel has been established for SCP data transfers  
on port 21796 to host zeus.rdhpcs.noaa.gov.  
  
PLEASE NOTE:  
=====  
You will need to reconfigure your SSH client
```

TUNNELLING – *Getting data from here to there*

Linux Example (continued)

Copying Data

To use the port tunnel for SCP from your host:

Template:

```
scp -P 21796 /local/path/to/file Daniel.Schornak@localhost:/remote/path/to/file  
or
```

```
scp -P 21796 Daniel.Schornak@localhost:/remote/path/to/file /local/path/to/file
```

(Windows PUTTY users will use pscp instead of scp)

IMPORTANT NOTE:

=====

ALWAYS USE '**localhost**' for the SCP commands so the port tunnel is used.

NESCC Factoid...

“localhost” <> “hostname”

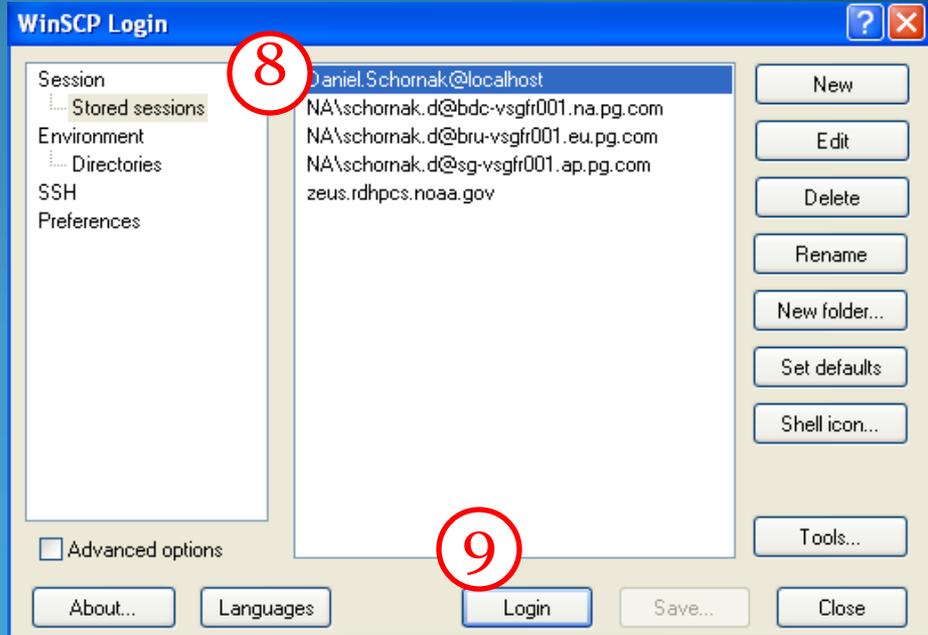
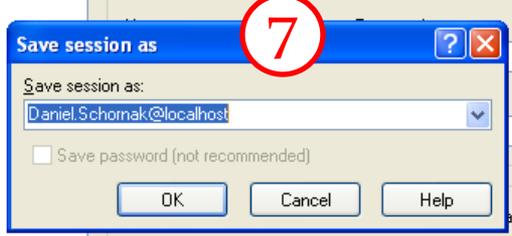
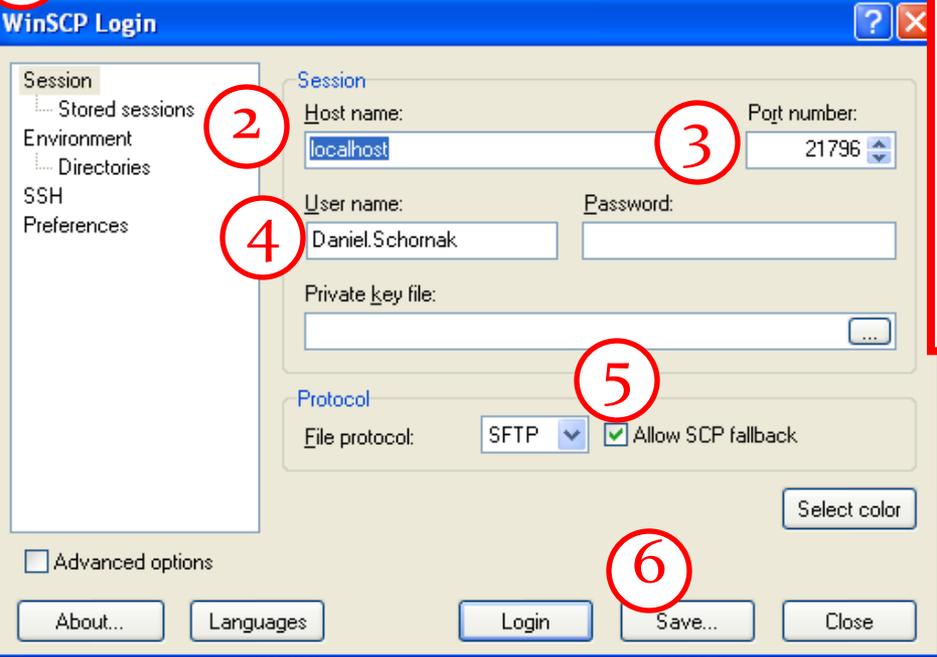
TUNNELLING – Getting data from here to there

WinSCP Example

1

Prerequisite: Active PuTTY session on must be running

1. Start WinSCP
2. In Session Window Host name type: **localhost**
3. Enter your NESCC-provided Local tunnel port number
4. Enter your “**User name**”
5. Select: “**Allow SCP fallback**”
6. Select: “**Save**”
7. Provide a name for your session
8. Select the session name
9. Select “**Login**”

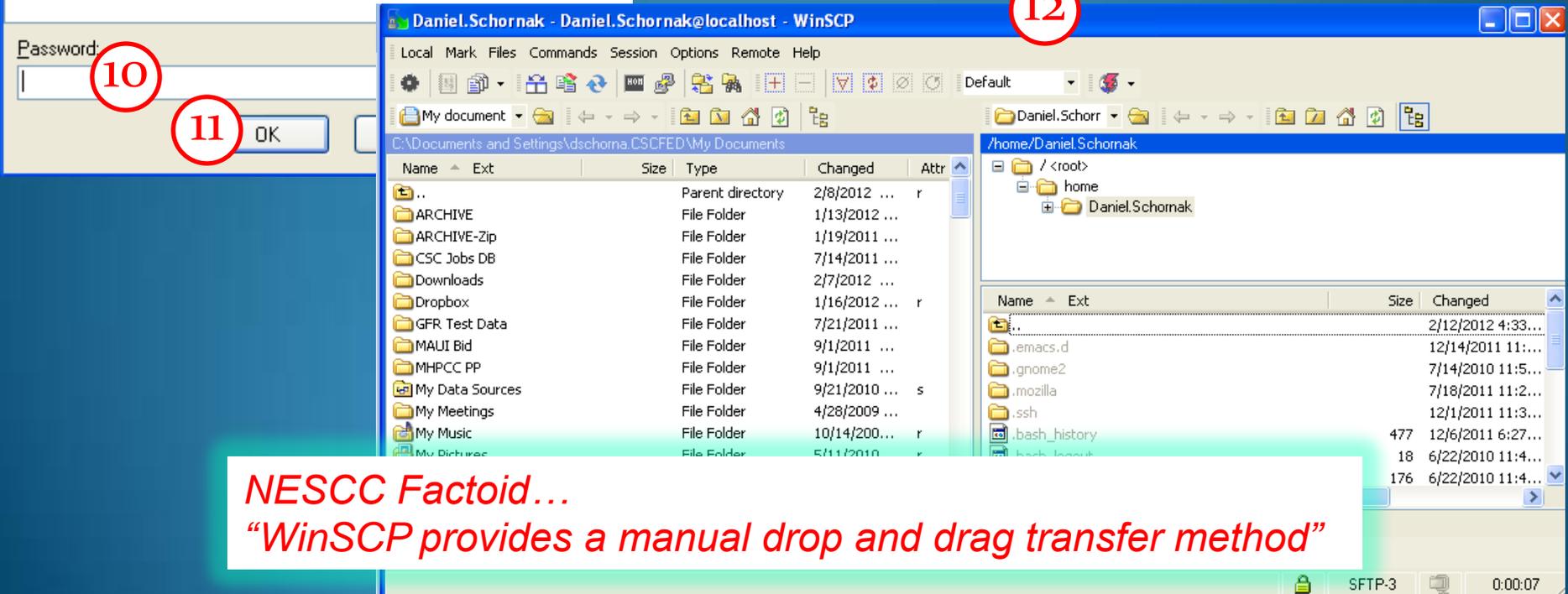


TUNNELLING – Getting data from here to there

WinSCP Example (continued)



10. Enter local NESCC passwd
11. Select "OK"
12. Upon successful login, WinSCP window appears



NESCC Factoid...

"WinSCP provides a manual drop and drag transfer method"

Data Movers – Getting data from here to there

DTN node: dtn1

Data Transfer Host (Preferred Approach) – *Inside noaa.gov*

Note: Requires Token Authentication

Prerequisite (on Zeus)

- Create your subdirectory in the appropriate /scratchX/portfolios/<portfolio>/< project>
Hint: Use “account_params” command to help determine the <portfolio> and <project>

Example Transfer

```
scp filex Daniel.Schornak@dtn1.fairmont.rdhpcs.noaa.gov:/scratch2/portfolios/BMC/nescmgmt/Daniel.Schornak
```

#Daniel Schornak will see the following prompt:

```
'Daniel.Schornak@dtn1.fairmont.rdhpcs.noaa.gov's password: <PIN+RSA token>
```

#Upon successful password entry, the DTN node is added to the “known hosts”

Warning: Permanently added 'dtn1.fairmont.rdhpcs.noaa.gov,140.90.206.58' (RSA) to the list of known hosts.

The file then transfers and reports the following:

```
filex                               100% 128MB 32.0MB/s 00:04
```

Jet account users

You can still access jetscp where Zeus is just another remote host.

https://jetdocs.rdhpcs.noaa.gov/wiki/index.php/Transferring_Files#Option_2:_jetscp

Data Movers – *Getting data from here to there*

Unattended Data Transfer – *inside .noaa.gov*

- Set up upon special request
- Transfers from known specific hosts inside .noaa.gov
- Transfers to known specific user names on Zeus
- Send a request to the help system explaining your requirements and the list of IP addresses from which the transfers will occur

Outbound transfers

- No special hosts, all front end nodes have been designed to support transfers
- If you need to transfer data as part of your workflow, submit those pieces of workflow to the service queue

“What if I need better transfers to Zeus from outside .noaa.gov?”

Please email the help system and let us know what you are trying to do. This will help to determine the best solution and course of action.

rdhpcs.zeus.help@noaa.gov

User Environment – Environment Variables

Environment Variable	Example Output (echo <Environment Variable>)	Description
\$HOME	/home/daniel.schornak	Typically , the initial directory after logging in
\$PATH	/usr/local/bin:/usr/local/X11/bin:/etc:/usr/etc:/usr/local/etc:.	Provides search path for shell commands. (User modifiable)
\$SHELL	/bin/tcsh	Current active UNIX shell for session (User modifiable) Available shells include: sh (bourne SHell); bash (Bourne-Again SHell); csH (C SHell); ksh (Korn SHell); tcsh (TC SHell); zsh – Z SHell
\$PWD	/home/daniel.schornak	Print Working Directory. Changing directory locations updates this environment variable
\$LOGNAME	daniel.schornak	Name of the user
\$MAIL	/var/spool/mail/daniel.schornak	Location of incoming mail
\$USER		Name of the user

User Environment – Environment Variables

<p>NCEP</p> <p>AUTHSTATE=files MANPATH=/opt/c3/man:/usr/sbin/rsct/man: TERM=xterm SHELL=/usr/bin/ksh SSH_CLIENT=140.90.206.41 OBJECT_MODE=64 MP_SHARED_MEMORY=0 SSH_TTY=/dev/pts/0 LOCPATH=/usr/lib/locale/locale-archive USER=wx15rrl ODMDIR=/etc/obd TVDSVRLAUNCHCMD=sshd A_z=! LOGNAME=daniel.schornak MAIL=/usr/spool/mail/daniel.schornak PATH=/usrx/local/bin:/usrx/local/sbin:/usrx/local/bin:/usrx/local/sbin:/usr/local/bin:/usr/local/sbin:/usr/bin:/usr/sbin:/opt/c3/bin:/opt/c3/sbin:/opt/sgi/sbin:/opt/sgi/bin MAIL=/var/spool/mail/Daniel.Schornak SHELL=/bin/tcsh LD_LIBRARY_PATH=/usr/local/globus/5.0.4/lib:/apps/torque/lib LIBPATH=/usr/local/globus/5.0.4/lib:/usr/lib/lib SHLIB_PATH=/usr/local/globus/5.0.4/lib GLOBUS_LOCATION=/usr/local/globus/5.0.4 SSH_CLIENT=140.90.206.41 33889 22 SSH_CONNECTION=140.90.206.41 33889 140.90.206.33 22 SSH_TTY=/dev/pts/5 TERM=xterm HOSTTYPE=x86_64-linux VENDOR=unknown OSTYPE=linux MACHTYPE=x86_64 SHLVL=1 PWD=/home/Daniel.Schornak GROUP=zeusgrp18100 HOST=fe1 REMOTEHOST=tfe1.fairmont.rdhpcs.noaa.gov HOSTNAME=fe1 MANPATH=/opt/c3/man:/usr/local/man:/opt/sgi/share/man LS_COLORS=rs=0:di=01;34:ln=01;36:mh=00:pi=40;33:so=01;35:do=01;35:bd=40;33;01:or=40;05;37;41:su=37;41:sg=30;43:ca=30;41:tw=30;42:ow=34;42:st=37;44:ex=01;32:*:tar=01;31:*:tgz=01;31:*: G_BROKEN_FILENAMES=1 LESSOPEN= /usr/bin/lesspipe.sh %s MOABHOMEDIR=/var/spool/moab TORQUEHOMEDIR=/var/spool/torque MODULESHOME=/usr/share/Modules MODULEPATH=/usr/share/Modules/modulefiles:/etc/modulefiles:/etc/modulefiles:/apps/modulefiles LOADEDMODULES= OSCAR_HOME=/opt/oscar C3_RSH=ssh -oConnectTimeout=10 -oForwardX11=no</p>	<p>ESRL</p> <p>USER=daniel.schornak LOGNAME=daniel.schornak HOME=/home/daniel.schornak PATH=/usr/local/bin:/usr/local/sbin:/usr/local/bin:/usr/local/sbin:/usr/local/etc.: MAIL=/var/spool/mail/daniel.schornak SHELL=/bin/tcsh SSH_CLIENT=140.172.21.140 SSH_CONNECTION=140.172.21.140 4343 140.172.21.140 SSH_TTY=/dev/pts/43 TERM=xterm HOSTTYPE=x86_64-linux VENDOR=unknown OSTYPE=linux MACHTYPE=x86_64 SHLVL=1 PWD=/home/daniel.schornak GROUP=csc HOST=fe5 REMOTEHOST=bastion-j LS_COLORS=no=00:fi=00:di=01;34:ln=01;36:mh=00:pi=40;33:so=01;35:do=01;35:bd=40;33;01:or=40;05;37;41:su=37;41:sg=30;43:ca=30;41:tw=30;42:ow=34;42:st=37;44:ex=01;32:*:tar=01;31:*:tgz=01;31:*: G_BROKEN_FILENAMES=1 LESSOPEN= /usr/bin/lesspipe.sh %s QTDIR=/usr/lib64/qt-3.3 QTINC=/usr/lib64/qt-3.3/include QTLIB=/usr/lib64/qt-3.3/lib MANPATH=/opt/toolwork INFOPATH=/usr/info:usr/share/info C_INCLUDE_PATH=/usr/include CPLUS_INCLUDE_PATH=/usr/include LIBRARY_PATH=/lib64:/usr/lib64 LD_LIBRARY_PATH=/opt/c3/lib:/usr/lib64:/usr/lib LD_RUN_PATH=/lib64:/usr/lib64 XAPPLRESDIR=/usr/lib/X11 MODULE_VERSION=3.2 MODULE_VERSION_STATUS=3.2 MODULESHOME=/opt/ncep MODULEPATH=versions: SGE_ROOT=/opt/sge/default TVDSVRLAUNCHCMD=sshd UDUNITS=/opt/udunits/ _LMFILES=/opt/modulefiles ENV=/home/daniel.schornak HOSTNAME=fe5 INPUTRC=/etc/inputrc</p>	<p>GFDL</p> <p>TERM=xterm HOME=/home/Philip.Holle SHELL=/bin/tcsh USER=Philip.Holle LOGNAME=Philip.Holle PATH=/home/gfdl/bin:/usr/local/bin:/usr/local/sbin:/usr/local/bin:/usr/local/sbin:/usr/bin:/usr/sbin:/opt/c3/bin:/opt/c3/sbin:/opt/sgi/sbin:/opt/sgi/bin MAIL=/var/spool/mail/Daniel.Schornak SHELL=/bin/tcsh LD_LIBRARY_PATH=/usr/local/globus/5.0.4/lib:/apps/torque/lib LIBPATH=/usr/local/globus/5.0.4/lib:/usr/lib/lib SHLIB_PATH=/usr/local/globus/5.0.4/lib GLOBUS_LOCATION=/usr/local/globus/5.0.4 SSH_CLIENT=140.90.206.41 33889 22 SSH_CONNECTION=140.90.206.41 33889 140.90.206.33 22 SSH_TTY=/dev/pts/5 TERM=xterm HOSTTYPE=x86_64-linux VENDOR=unknown OSTYPE=linux MACHTYPE=x86_64 SHLVL=1 PWD=/home/Philip.Holle GROUP=y HOST=pp054 REMOTEHOST=pp054 LANG=en_US LC_TIME=C HOSTNAME=pp054 LD_LIBRARY_PATH=/usr/local/globus/5.0.4/lib:/usr/lib/lib MANPATH=/usr/local/man:/opt/sgi/share/man MODULE_VERSION=3.2 MODULE_VERSION_STATUS=3.2 MODULESHOME=/opt/ncep MODULEPATH=/usr/share/Modules/modulefiles:/etc/modulefiles:/etc/modulefiles:/apps/modulefiles LOADEDMODULES= OMP_NUM_THREADS=1 TMPDIR=/vftmp/Philip.Holle FTMPDIR=/vftmp/Philip.Holle ARCHIVE=/archive XENVIRONMENT= XAUTHORITY=/home/Philip.Holle/.Xauthority XAPPLRESDIR=/usr/lib/X11</p>	<p>NESCC</p> <p>LANG=en_US.UTF-8 USER=Daniel.Schornak LOGNAME=Daniel.Schornak HOME=/home/Daniel.Schornak PATH=/usr/bin:/bin:/usr/sbin:/sbin:/usr/local/globus/5.0.4/bin:/usr/local/globus/5.0.4/bin:/opt/c3/bin:/opt/c3/sbin:/opt/sgi/sbin:/opt/sgi/bin MAIL=/var/spool/mail/Daniel.Schornak SHELL=/bin/tcsh LD_LIBRARY_PATH=/usr/local/globus/5.0.4/lib:/apps/torque/lib LIBPATH=/usr/local/globus/5.0.4/lib:/usr/lib/lib SHLIB_PATH=/usr/local/globus/5.0.4/lib GLOBUS_LOCATION=/usr/local/globus/5.0.4 SSH_CLIENT=140.90.206.41 33889 22 SSH_CONNECTION=140.90.206.41 33889 140.90.206.33 22 SSH_TTY=/dev/pts/5 TERM=xterm HOSTTYPE=x86_64-linux VENDOR=unknown OSTYPE=linux MACHTYPE=x86_64 SHLVL=1 PWD=/home/Daniel.Schornak GROUP=zeusgrp18100 HOST=fe1 REMOTEHOST=tfe1.fairmont.rdhpcs.noaa.gov HOSTNAME=fe1 MANPATH=/opt/c3/man:/usr/local/man:/opt/sgi/share/man LS_COLORS=rs=0:di=01;34:ln=01;36:mh=00:pi=40;33:so=01;35:do=01;35:bd=40;33;01:or=40;05;37;41:su=37;41:sg=30;43:ca=30;41:tw=30;42:ow=34;42:st=37;44:ex=01;32:*:tar=01;31:*:tgz=01;31:*: G_BROKEN_FILENAMES=1 LESSOPEN= /usr/bin/lesspipe.sh %s MOABHOMEDIR=/var/spool/moab TORQUEHOMEDIR=/var/spool/torque MODULESHOME=/usr/share/Modules MODULEPATH=/usr/share/Modules/modulefiles:/etc/modulefiles:/etc/modulefiles:/apps/modulefiles LOADEDMODULES= OSCAR_HOME=/opt/oscar C3_RSH=ssh -oConnectTimeout=10 -oForwardX11=no</p>
--	--	--	--

Introduction to User Environment, Policies, Quotas, and Environmental Variables

Drafted Policies

- Login Node Usage Policy
- Cron Usage Policy
- Home File System Usage Policy
- High Performance Storage Usage Policy
- Filesystem Backup and Data Retention Policy
- Maximum Job Length Policy

Introduction to User Environment, Policies, Quotas, and Environmental Variables

Policy – Login Node Usage Policy (Draft)

Policy Name – Login Node Usage Policy (Draft)

The Zeus login (“frontend”) nodes provide access to the rest of the cluster. They are intended for code and batch job management tasks, not for computation.

Login nodes should ONLY be used for tasks similar to the following:

- Editing and compiling code
- Only perform simple tasks on login nodes
- Perform administrative tasks
- Run NO Compute jobs

Tasks that do not fit into the above categories should be run via the batch system. Processes that use a significant amount of resources, especially if they execute regularly, are better run via the batch system. There are two ways the user can do this:

- Create a batch script and submit it as a compute or serial job
- Use a dedicated node or nodes in an interactive job session

For further details visit:

https://nescdocs.rdhpcs.noaa.gov/wiki/index.php/Login_Node_Usage_Policy

Introduction to User Environment, Policies, Quotas, and Environmental Variables

Policy – Cron Usage Policy (Draft)

Policy Name – Cron Usage Policy (Draft)

The Cron service is provided for users to launch time sensitive jobs. Any cron jobs will be started on the service/login nodes. Therefore any policies that exist on the service nodes should be applied to the cron jobs.

Users manage and run their own crontabs

For further details visit:

[https://nescdocs.rdhpcs.noaa.gov/wiki/index.php/Cron Usage Policy](https://nescdocs.rdhpcs.noaa.gov/wiki/index.php/Cron_Usage_Policy)

Introduction to User Environment, Policies, Quotas, and Environmental Variables

Policy – Home File System Usage Policy (Draft)

Policy Name – Home File System Usage Policy (Draft)

The home filesystem is designed for the following operations:

- Ed `/home` is intended for source code and critical components that
- St `/home` cannot be easily replicated
- Storing user environment configuration files

The home file `/home` is backed up regularly `/home` has a snapshot capability to ensure rapid retrieval of accidentally deleted files.

Operations that should NOT be performed on the home filesystem:

- Storing `/home` NOT intended for model input/output data or parallel I/O
- Parallel IO of any kind.

Please use the high performance storage filesystems for these types of operations.

The default quota `Default quota for user's /home directory is 5GB` space will be considered on a case-by-case basis.

For further details visit:

https://nescdocs.rdhpcs.noaa.gov/wiki/index.php/Home_File_System_Usage_Policy

Introduction to User Environment, Policies, Quotas, and Environmental Variables

Policy – High Performance Storage Usage Policy (Draft)

Policy Name – High Performance Storage Usage Policy (Draft)

The high performance storage (HPS) filesystems (/scratch₁ and /scratch₂) are fast, parallel, and scalable. /scratch is intended for model input/output data and parallel I/O. This policy describes how these filesystems are maintained.

- The HPS /scratch is allocated on a project basis
- Quotas on /scratch are enforced on a per project basis
- These filesystems are scratch and are NOT backed up
 - Users on /scratch is NOT backed up or purged
- The HPS filesystems will not be scrubbed
 - If project /scratch cleanup is the responsibility of the project

For further details visit:

https://nescdocs.rdhpcs.noaa.gov/wiki/index.php/High_Performance_Storage_Usage_Policy

Introduction to User Environment, Policies, Quotas, and Environmental Variables

Policy – Filesystem Backup and Data Retention Policy (Draft)

Policy Name – Filesystem Backup and Data Retention Policy (Draft)

All of the file systems with the exception of /home and the HSMS are considered scratch file systems. We want users to be aware of the risks with **Scratch filesystems are NOT backed up** in any way. While we do our best to ensure the reliability of those file systems, they are not perfect and there is a small risk that data could be lost without any possibility of recovery.

Much of the data generated on the scratch filesystems may be difficult, labor-intensive, or resource-intensive to recreate. In this case, we strongly recommend **Save your important results to the HSMS regularly** at a reasonable frequency based on your work structure. But you should save data to the HSMS at a frequency of no less than weekly.

Please do not save **HSMS is a finite storage resource and will have quotas applied. Don't save multiple versions of the same data. Bundle your data with tar, cpio or htar** limited resources. You should not save multiple versions of the same data. Bundle your data with tar, cpio or htar feasible using tools such as tar or cpio.

Finally, labor intensive files **Don't leave important single copy data on Scratch filesystems** and to build executable programs can be built on the scratch filesystems but they should not be built on the scratch filesystems.

Snapshots are created on the /home file system nightly and are kept for two weeks back. Within the two week period, files on /home may be restored from the snapshot dir **/home snapshots good for two weeks; backups good for 6 months** approximately 6 months. Requests to recover data from a Disaster Recovery backup will be evaluated on a case by case basis.

For further details visit:

https://nescdocs.rdhpcs.noaa.gov/wiki/index.php/High_Performance_Storage_Usage_Policy

Introduction to User Environment, Policies, Quotas, and Environmental Variables

Policy – Maximum Job Length Policy (Draft)

Policy Name – Maximum Job Length Policy (Draft)

The maximum job length for jobs on the NESCC systems is 8 hours. This policy has been developed after assessing the current system, and reducing risk of losing too many CPUhours from failed jobs or system interruptions. Default queue wallclock time is 30 minutes; Maximum wallclock time is 8 hours.

If you need to run longer than 8 hours, checkpoint your application and resubmit the job to the batch system.

For further details visit:

https://nescdocs.rdhpcs.noaa.gov/wiki/index.php/Maximum_Job_Length_Policy

Introduction to User Environment, Policies, Quotas, and Environmental Variables

Proposed Zeus Frontend Limits		Description
memlock(soft)	4194304 (KB) [0.5GB]	max locked-in-memory address space (KB)
memlock(hard)	8388608 (KB) [1GB]	max locked-in-memory address space (KB)
nofile (soft/hard)	6400/64000	max number of open files
locks (soft/hard)	64/1024	max number of file locks the user can hold
nproc (soft/hard)	64/512	max number of processes
cpu (soft/hard):	100/2000	max CPU time (MIN)
maxlogins (soft/hard):	20/20	max number of logins for this user

Introduction to User Environment, Policies, Quotas, and Environmental Variables

In Practice – Tape Storage Access

Tape Storage

The tape storage assets will not be directly mounted to the login or compute nodes. Access is provided through custom scripts (htar and hsi) that will permit the transfer of data to and from the tape storage server.

NESCC Factoid...

“Current methods to use the tape storage are hsi and htar. Other methods will be provided prior to Zeus going into production.”

Introduction to User Environment, Policies, Quotas, and Environmental Variables

Command location: /apps/hpss/bin/hsi.ksh
alias hsi /apps/hpss/bin/hsi.ksh

```
Daniel.Schornak@fe4:~$ hsi
[connecting to hpsscore1.fairmont.rdhpcs.noaa.gov/1217]
*****
* Welcome to the NESCC High Performance Storage System *
* *
* Current HPSS version: 7.3.2 Patch 2 *
* *
* Contact Information: *
* *
* Skylar Nelson <snelson@ebi-llc.com> *
* John Moffatt <jmoffatt@ebi-llc.com> *
* *
* Please Submit Helpdesk Request to *
* rdhpcs.hpss.help@noaa.gov *
* *
* Announcements: *
*****
Username: Daniel.Schornak UID: 10496 Acct: 10496(10496) Copies: 1
[hpsscore1]/NCEPDEV/hpssuser/g01/Daniel.Schornak->
[Daniel.Schornak@fe4 ~]$
```

```
Daniel.Schornak@tfel:~$ hsi -h
[connecting to hpsscore1.fairmont.rdhpcs.noaa.gov/1217]
hsi: missing hostname parameter
Usage: hsi -help. (or -?).
-----
hsi [-a acct_id|acct_name] [-A authmethod] [-c krb_cred_file] [-d level] [-e] [-G globus proxy path]
[-h host[/port]] [-k.keytabfile] [-l loginname] [-O listingFile] [-o] [-P] [-p port] [-s site]
[-q] [-v] [cmds]
Parameters:
-a acct_id | acct_name - specifies the HPSS account ID or account name to set
after login completes. This will be used for all new file creations
-A authmethod - authentication method. Case-insensitive legal method names are:
"combo", "keytab", "ident", "gsi", "local"
-c krb_cred_file - pathname to use for Kerberos credentials cache file
-d debug_level - debug message level (0-5); default is 0
-e - command echo flag. Echos lines read from <IN> file(s) to the listable output file
-h host - specifies host name or IP address of the HPSS server, and optionally,
the port on which to connect
-k keytabfile - specifies pathname to DCE keytab file
-l loginname - specifies login name to use
For kerberos, this is usually of the form "name@realm"
-O listingFile - specifies filename to contain all listable output, error messages, etc
This option is intended for use by programs that run hsi as a child process
and internally disables verbose (-v) mode, and sets quiet (-q) mode. (This can
be overridden by specifying the -v or -q parameters after the -O parameter)
-o (root only) - override <no-login> setting
-P ("popen" flag) - specifies that HSI is being run via popen (as a child process).
All messages (listable output, error message) are written to stdout.
HSI may not be used to pipe output to stdout if this flag is specified.
-p port - specifies the port number to use when connecting to the HPSS server
If -p is specified, then the optional port should be omitted from the -h
option, if -h is specified
-q - specifies "quiet" mode. Suppresses login message, file transfer progress messages, etc.
name must match one of
's private .hsirc file
```

NESCC Factoid...

"Similar to ftp commands...the hsi command is used to move files to and from the HPSS."

Introduction to User Environment, Policies, Quotas, and Environmental Variables

```
Daniel.Schornak@fe2:~  
[Daniel.Schornak@fe2 ~]$ htar -h  
Using fe2-10 for data hostname  
[connecting to hpsscore1.fairmont.rdhpcs.noaa.gov/1217]  
ERROR: No action specified (-c, -K, -t, -x, -X).  
Usage:  
  
htar  -{c|D|K|t|U|x|X} -f Archive [-?] [-B] [-E] [-h] [-H opt[:opt...]  
      [-d debuglevel] [-I {IndexFile | .suffix}] [-L inputlist]  
      [-M maxfiles] [-m] [-n days[:hours]] [-O] [-o] [-p] [-q]  
      [-v] [-V [-w [-Y auto | [Archive COS ID][:Index File COS ID]]  
      [-S bufsize] [-T Max Threads] [Filespec | Directory ...]  
HTAR: HTAR FAILED  
[Daniel.Schornak@fe2 ~]$
```

NESCC Factoid...

“Similar to tar commands...the htar command is used to compress and package files into one file in order to minimize storage requirements – But then moves this file to HPSS storage.”

Introduction to User Environment, Policies, Quotas, and Environmental Variables



Recommended Exercises

1. Log into TDS or Zeus
 - a. Try using PuTTY (Windows Environment)
 - b. Try using SSH (Linux Environment)
2. Get to know your session environmental variables (*"printenv"*)
3. Review and Explore the User Environment
4. Set up an SSH Tunnel between your system and TDS or Zeus
5. Copy files to the /scratch1 or /scratch2 volumes via DTNs
6. Knowing the Limitations – Established Policies and Quotas
 - a. Determine available files systems (*"df"*)
 - b. Locate posted policies and quotas

Programming Environment – *Environment Variables*

Environment Variable	Example Output (echo <Environment Variable>)	Description
\$LD_LIBRARY_PATH	/opt/java/jdk1.6.0_04//lib:/opt/udunits/2.1.15/lib:/opt/papi/4.1.0/lib:/opt/ncl/5.2.0_bin/lib:/opt/hdf5/1.8.3-intel/lib:/opt/netcdf/3.6.3-intel/lib:/opt/intel/Compiler/11.1/072//idb/lib/intel64:/opt/intel/Compiler/11.1/072//mkl/lib/em64t:/opt/intel/Compiler/11.1/072//lib/intel64:/lib:64/usr/lib:64/usr/X11R6/lib64:/usr/local/lib64:/opt/sge/default/lib/lx26-amd64:/usr/local/lib64	Base path for resolving library paths for applications using Shared Objects and linkers
\$LIBRARY_PATH	/lib64:/usr/lib64:/usr/X11R6/lib64:/usr/local/lib64:/usr/local/lib64	Provides search locations for resolving interactive and script command entries. (User modifiable)
\$SHELL	/bin/tcsh	Current active UNIX shell for session (User modifiable) Available shells include: sh (bourne SHell); bash (Bourne-Again SHell); csh (C SHell); ksh (Korn SHell); tcsh (TC SHell); zsh (Z SHell)
\$PWD	/home/Daniel.Schornak	Print Working Directory. Changing directory locations updates this environment variable
\$LOGNAME	daniel.schornak	Name of the user
\$MAIL	/var/spool/mail/daniel.schornak	Location of incoming mail
\$USER	Daniel.Schornak	Name of the user

Programming Environment – Alias command

Alias command provides a simplified way of performing compound commands

```
Daniel.Schornak@fe1:~  
[Daniel.Schornak@fe1 ~]$ alias  
l.      ls -d .* --color=auto  
ll      ls -l --color=auto  
ls      ls --color=auto  
module (set _prompt="$prompt";set prompt=""  
h !*`; set _exit=$status; set prompt="$_prom  
$_exit;)  
vi      vim  
which   alias | /usr/bin/which --tty-only --  
tilde  
[Daniel.Schornak@fe1 ~]$
```

```
Daniel.Schornak@fe1:~  
[Daniel.Schornak@fe1 ~]$ /  
 2 20:57 qmgr  
 3 21:01 showq  
 5 21:01 showq -v -v  
 6 21:01 man showq  
 7 21:03 mshow  
 8 21:04 pbsnodes  
 9 21:04 showbf  
10 21:04 showbf -v -v  
11 21:06 qstat  
12 21:06 qstat -v -v  
14 21:06 qstat -f  
15 21:06 man qstat  
16 22:10 ssh ftel  
18 22:10 ssh tfel  
19 22:10 ping tfel  
20 22:11 alias  
23 22:11 vi .cshrc  
24 22:12 vi .bashrc  
25 22:12 chmod 644 .cshrc  
26 22:12 . .cshrc  
27 22:12 source .cshrc  
28 22:12 /  
[Daniel.Schornak@fe1 ~]$
```

Example:

At command line type: alias / history

Now display shell history by typing: /



Note:

Add the above entry to .cshrc and it will be available at shell instantiation

Result from using new aliased command

Programming Environment – *Editors*

Available Editors	Learn More	Description
ed (a.k.a. red)	ed --help red --help	Line editor
vi	vi --help	Visual Interface (Note: vi is aliased to vim at NESCC)
emacs	emacs --help	Emacs is the extensible, customizable, self-documenting real-time display editor. This Info file describes how to edit with Emacs and some of how to customize it; it corresponds to GNU Emacs version 23.1.
rvi (a.k.a. vim; rview)	rvi --help vim --help rview --help	Vi IMproved, a programmer's editor
ex	ex --help	Line editor or VIM editor capability

Introduction to Programming Environment

General Compiler Discussion

Compilers	Intel * (<i>module load intel</i>)	Portland Group (<i>module load pgi</i>)
CC	icc	pgcc
F77	ifort	pgf77
F90	ifort	pgf90
C++	icpc	pgCC

*Intel compilers are the primary compilers on Zeus

Introduction to Programming Environment

Numerical Libraries Discussion

Source	Package	Associated Libraries
Intel	Math Kernel Library (MKL)	BLAS, LAPACK, PARDISO, FFT, FFTW, ScaLAPACK, Vector Math Library (VML), Vector Statistical Library (VSL), Summary Statistics Library (SSL)
PGI	PGI Math libraries	LAPACK, BLAS, FFT, Cluster FFT
SGI	Message Passing Toolkit (MPT)	Message Passing Toolkit (MPT) is a software package that supports interprocess data exchange for applications that use concurrent, cooperating processes on a single host or on multiple hosts. Data exchange is done through message passing, which is the use of library calls to request data delivery from one process to another or between groups of processes.

Many codes may use IBM's ESSL and, in particular, FFT routines.
ESSL is not available for the x86_64 platform.

Module Commands

- *module help*
- *module avail*
- *module whatis*
- *module load*
- *module list*
- *module unload*
- *module switch*
- *module show*

NESCC Factoid...

“Modules will continue to be refined during the Zeus acceptance period (through March 1st). After that period, defaults will be finalized. Alternate versions will be accessible over time as needed through different module titles.”

Module Command - “*module --help*”

```
[daniel.schornak@fe2 ~]$ module --help

Modules Release 3.2.6 2007-02-14 (Copyright GNU GPL v2 1991):

Usage: module [ switches ] [ subcommand ] [subcommand-args ]

Switches:
  -H|--help           this usage info
  -V|--version        modules version & configuration options
  -f|--force          force active dependency resolution
  -t|--terse          terse      format avail and list format
  -l|--long           long       format avail and list format
  -h|--human          readable format avail and list format
  -v|--verbose        enable  verbose messages
  -s|--silent         disable verbose messages
  -c|--create         create  caches for avail and apropos
  -i|--icase          case   insensitive
  -u|--userlvl <lvl> set user level to (nov[ice],exp[ert],adv[anced])

Available SubCommands and Args:
+ add!load           modulefile [modulefile ...]
+ rm!unload          modulefile [modulefile ...]
+ switch!swap        [modulefile1] modulefile2
+ display!show       modulefile [modulefile ...]
+ avail              [modulefile [modulefile ...]]
+ use [-a|--append]  dir [dir ...]
+ unuse              dir [dir ...]
+ update
+ refresh
+ purge
+ list
+ clear
+ help               [modulefile [modulefile ...]]
+ whatis             [modulefile [modulefile ...]]
+ apropos!keyword   string
+ initadd            modulefile [modulefile ...]
+ initprepend        modulefile [modulefile ...]
+ initrm             modulefile [modulefile ...]
+ initswitch         modulefile1 modulefile2
+ initlist
+ initclear
```

Sample Output “*module --help*”

Module Commands – “module avail”

```

Daniel.Schornak@fe6:~$ module avail

----- /usr/share/Modules/modulefiles -----
chkfeature  module-cvs  modules      null          perfcatcher
dot          module-info  mpt/2.05     perfboost     use.own

----- /apps/modulefiles -----
adaptive/6.1.0          intel/12-12.0.4.191 (default)
adaptive/6.1.3 (default)  intel/12-12.1.0_spl.6.233
bbcp/10.08.29.00.0 (default)  matlab/r2011b
bbftp/client/3.2.0          mcidas/1.01 (default)
bbftp/server/3.2.0         ncl/6.0.0 (default)
cnvgrib/1.2.2 (default)     nco/4.0.8 (default)
esmf/4.0.0r2 (default)     netcdf/3.6.3 (default)
g2clib/1.2.2 (default)     netcdf/4.1.3
g2lib/1.2.2 (default)     netcdf/4.1.3-gnu
grads/2.0.1 (default)     netcdf/4.1.3-intel
grads/2.0.a9              netcdf/4.1.3-pgi
gt/5.0.4 (default)        netcdf/test
hdf/4.2.6 (default)       netcdf4/python-0.9.7 (default)
hdf5/1.8.7 (default)      numpy/1.6.1 (default)
heirloom/cpio (default)   petsc/3.1-p8 (default)
hpss/hpss                  pgi/11.10 (default)
i7z/0.27 (default)        pgi/11.6
icc/12-12.0.4.191         pgi/11.6.orig
icc/12-12.1.0_spl.6.233   scipy/0.9.0 (default)
icc/12.1.0.233            tau/2.20.2 (default)
idl/idl/8.1                test/1
ifc/12-12.0.4.191         test/test
ifc/12-12.1.0_spl.6.233   totalview/8.9.1 (default)
imkl/12-12.0.4.191       udunits/1.12.11 (default)
imkl/12-12.1.0_spl.6.233  w3lib/2.0 (default)
impi/4.0.3.008            workflowmgr/0.99.152 (default)
[Daniel.Schornak@fe6 ~]$

```

Sample Output “module avail”

```

Daniel.Schornak@fe1:~$ module -l avail

-----+-----+ Versions +-+ Last mod. -----
/usr/share/Modules/modulefiles:
chkfeature      2011/10/09  5:25:57
dot             2009/12/09  16:22:52
module-cvs     2009/12/09  16:22:52
module-info    2009/12/09  16:22:52
modules        2009/12/09  16:22:52
mpt/2.05       2011/10/20  10:08:29
null           2009/12/09  16:22:52
perfboost      2011/10/20  10:58:17
perfcatcher    2011/10/20  10:46:04
use.own        2009/12/09  16:22:52

/etc/modulefiles:
/etc/modulefiles:

/apps/modulefiles:
adaptive/6.1.0          2011/12/01  13:01:34
adaptive/6.1.3          default    2012/01/13  17:03:52
bbcp/10.08.29.00.0     default    2011/12/01  13:01:34
bbftp/client/3.2.0     2011/12/01  13:01:34
bbftp/server/3.2.0     2011/12/01  13:01:34
cnvgrib/1.2.2          default    2011/12/01  13:01:34
esmf/4.0.0r2           default    2011/12/01  13:01:34
g2clib/1.2.2           default    2011/12/01  13:01:34
g2lib/1.2.2            default    2011/12/01  13:01:34
grads/2.0.1            default    2012/02/06  21:17:38
grads/2.0.a9           2011/12/01  13:01:34
gt/5.0.4               default    2011/12/01  13:01:34
hdf/4.2.6              default    2011/12/01  13:01:34
hdf5/1.8.7             default    2011/12/01  13:01:34
heirloom/cpio          default    2011/12/01  13:01:34
hpss/hpss               2012/01/30  13:12:01
i7z/0.27               default    2011/12/01  13:01:34
icc/12-12.0.4.191      2012/02/14  17:28:47
icc/12-12.1.0_spl.6.233 2012/02/14  17:28:47
icc/12.1.0.233         2012/02/14  17:28:47
idl/idl/8.1            2011/12/01  13:01:34
ifc/12-12.0.4.191     2012/02/14  17:29:20
ifc/12-12.1.0_spl.6.233 2012/02/14  17:29:20
imkl/12-12.0.4.191    2012/02/14  17:30:48

```

Sample Output “module -l avail”

Module Commands – “module whatis <module>”

```

cit : loads the default CIT management environment
cuda/2.0 : loads the CUDA development environment
cuda/2.1 : loads the CUDA development environment
cuda/2.1beta : loads the CUDA development environment
cuda/2.2 : loads the CUDA development environment
cuda/3.1 : loads the CUDA development environment
cuda/3.2.16 : loads the CUDA development environment
cuda/4.0.17 : loads the CUDA development environment
dot : adds . to your PATH
gams/23.7.1 : loads the path to GAMS
gempak/5.11.4 : loads the Gempak environment
gempak/6.2.0 : loads the Gempak environment
hdf4/4.2.5-intel : loads the HDF4 4.2.5-intel
hdf4/4.2r3-intel : loads the HDF4 4.2r3-intel
hdf4/4.2r3-lahey : loads the HDF4 4.2r3-lahey
hdf4/4.2r3-pgi : loads the HDF4 4.2r3-pgi
hdf5/1.8.3 : loads the HDF5 library
hmpp/2.4.2 : loads the HMPP Compiler
icc/11.1.038 : loads the Intel C/C++
icc/11.1.072 : loads the Intel C/C++
icc/11.1.073 : loads the Intel C/C++
icc/2011.2.137 : loads the Intel C/C++
ifort/11.1.038 : loads the Intel C/C++
impi/4.0.0.017 : loads the MUAPICH2 environment
intel/11.1.038 : loads the Intel Compiler
intel/11.1.072 : loads the Intel Compiler
intel/11.1.073 : loads the Intel Compiler
intel/2011.2.137 : loads the Intel Compiler
jet-tools : loads the default wJet environment
lahey/8.00a : loads the Lahey Compiler
lahey/8.10b : loads the Lahey Compiler
lf95/8.00a : loads the Lahey Fortran
lf95/8.10a : loads the Lahey Fortran
lf95/8.10b : loads the Lahey Fortran
mathlibs/fftw : loads the FFTW library
module-cvs : get most recent module
module-info : returns all various module information
modules : loads the modules environment
mvapich2/1.4.1-intel-11.1 : loads the MUAPICH2 environment
mvapich2/1.4.1-lahey : loads the MUAPICH2 environment
mvapich2/1.4.1-pgi : loads the MUAPICH2 environment
mvapich2/1.5-intel-11.1 : loads the MUAPICH2 environment
mvapich2/1.5-test-intel-11.1 : loads the MUAPICH2 environment
mvapich2/1.5.1-intel-11.1 : loads the MUAPICH2 environment
mvapich2/1.5.1-pgi : loads the MUAPICH2 environment
mvapich2/1.6-intel-11.1 : loads the MUAPICH2 environment
mvapich2/1.6-pgi : loads the MUAPICH2 environment
ncl/5.2.0 : loads the NCAR Graphics library
ncl/5.2.0-intel : loads the NCAR Graphics library
ncl/5.2.0-pgi : loads the NCAR Graphics library
nco/3.9.6 : loads the NCO environment
nco/4.0.1 : loads the NCO environment
netcdf/3.6.3 : loads the NETCDF library
netcdf/3.6.3-shared : loads the NETCDF shared library
netcdf/4.0.1 : loads the NETCDF library
netcdf/4.1.1 : loads the NETCDF library
netcdf/4.1.1-intel : loads the NETCDF shared library
netcdf/4.1.1-shared : loads the NETCDF shared library
null : does absolutely nothing
openmpi/1.3.3 : loads the OpenMPI library
openmpi/1.4.1 : loads the OpenMPI library
openmpi/1.4.1-intel-11.1 : loads the OpenMPI library
openmpi/1.4.1-lahey : loads the OpenMPI library
openmpi/1.4.1-pgi : loads the OpenMPI library
openmpi/1.4.2-intel : loads the OpenMPI library
openmpi/1.4.2-lahey : loads the OpenMPI library
openmpi/1.4.2-pgi : loads the OpenMPI library
openmpi/1.4.3-intel : loads the OpenMPI library
openmpi/1.4.3-lahey : loads the OpenMPI library
openmpi/1.4.3-pgi : loads the OpenMPI library
openmpi/1.7ft_a2-intel : loads the OpenMPI library
papi/4.1.0 : loads PAPI
pgcc/10.6 : loads the PGI compiler environment
pgcc/10.8 : loads the PGI compiler environment
pgcc/10.9 : loads the PGI compiler environment
pgcc/11.1 : loads the PGI compiler environment
pgcc/11.7 : loads the PGI compiler environment
pgcc/9.0-2 : loads the PGI compiler environment
pgi/10.6 : loads the PGI Compiler environment
pgi/10.8 : loads the PGI Compiler environment
pgi/10.9 : loads the PGI Compiler environment
pgi/11.1 : loads the PGI Compiler environment
pgi/11.7 : loads the PGI Compiler environment
pgi/9.0-2 : loads the PGI Compiler environment
sge : loads the SGE environment
sms/2.9.0-intel-9.1 : loads the SMS environment for Intel 9.1/MUAPICH2-1.0
sms/2.9.0-pgi-7.1-3-mvapich2-1.0.3 : loads the SMS environment for Intel 9.1/MUAPICH2-1.0
torque : loads the Torque environment
totalview/8.8.0-1 : loads the TotalView debugging environment
uberftp/2.7 : loads the Gempak environment
udunits/2.1.15 : loads the Udunits environment
use.own : adds your own modulefiles directory to MODULEPATH
wgrrib/1.8.1.0d : loads the path to wgrrib
wgrrib2/1.9.2c : loads the path to wgrrib2
wjet : loads the default wJet environment

```

Sample Output – “module whatis <module>”

Module Commands – “module load”

```
Daniel.Schornak@fe6:~$ printenv
Before loading modules
LD_LIBRARY_PATH: /usr/local/globus/5.0.4/lib:/usr/local/globus/5.0.4/lib:/apps/moab/default/lib:/apps/torque/default/lib:/apps/moab/default/lib:/apps/torque/default/lib
LIBPATH: /usr/local/globus/5.0.4/lib:/usr/local/globus/5.0.4/lib:/usr/lib:/lib
PATH: /usr/lib64/qt-3.3/bin:/usr/local/bin:/bin:/usr/bin:/usr/local/globus/5.0.4/bin:/usr/local/globus/5.0.4/bin:/opt/c3/bin:/apps/moab/default/moab/tools:/apps/moab/default/bin:/apps/torque/default/bin:/apps/gold/default/bin:/apps/gold/default/sbin:/opt/sgi/sbin:/opt/sgi/bin:/opt/c3/bin:/apps/moab/default/moab/tools:/apps/moab/default/bin:/apps/torque/default/bin:/apps/gold/default/bin:/apps/gold/default/sbin:/opt/sgi/sbin:/opt/sgi/bin
MANPATH: /opt/c3/man:/apps/moab/default/man:/apps/torque/default/man:/usr/share/man:/opt/sgi/share/man:/opt/c3/man:/apps/moab/default/man:/apps/torque/default/man:/usr/share/man:/opt/sgi/share/man

Loading module: module load intel ← Loading intel module

After loading intel module
LD_LIBRARY_PATH: /apps/intel/composerxe-2011.4.191/mkl/lib/intel64:/apps/intel/composerxe-2011.4.191/composerxe-2011.4.191/compiler/lib/intel64:/usr/local/globus/5.0.4/lib:/usr/local/globus/5.0.4/lib:/apps/moab/default/lib:/apps/torque/default/lib:/apps/moab/default/lib:/apps/torque/default/lib
LIBPATH: /usr/local/globus/5.0.4/lib:/usr/local/globus/5.0.4/lib:/usr/lib:/lib
PATH: /apps/intel/composerxe-2011.4.191/composerxe-2011.4.191/bin/intel64:/usr/lib64/qt-3.3/bin:/usr/local/bin:/bin:/usr/bin:/usr/local/globus/5.0.4/bin:/usr/local/globus/5.0.4/bin:/opt/c3/bin:/apps/moab/default/moab/tools:/apps/moab/default/bin:/apps/torque/default/bin:/apps/gold/default/bin:/apps/gold/default/sbin:/opt/sgi/sbin:/opt/sgi/bin:/opt/c3/bin:/apps/moab/default/moab/tools:/apps/moab/default/bin:/apps/torque/default/bin:/apps/gold/default/bin:/apps/gold/default/sbin:/opt/sgi/sbin:/opt/sgi/bin
MANPATH: /apps/intel/composerxe-2011.4.191/man/en_US:/opt/c3/man:/apps/moab/default/man:/apps/torque/default/man:/usr/share/man:/opt/sgi/share/man:/opt/c3/man:/apps/moab/default/man:/apps/torque/default/man:/usr/share/man:/opt/sgi/share/man
[Daniel.Schornak@fe6 ~]$
```

Basic Environment

← Loading intel module

Enhanced Environment

Sample Outputs from “printenv” ...Before and After “module load intel”

Module Commands

At Log in...

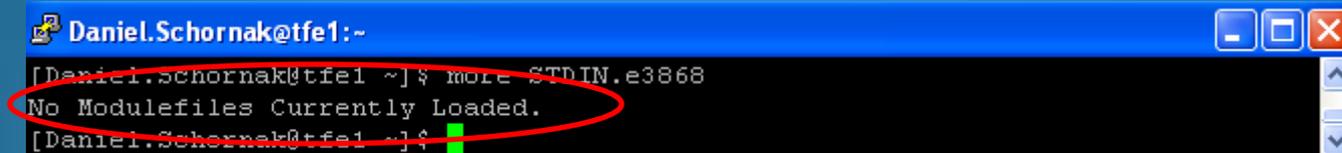
NESCC Factoid...

“Modules are not automatically loaded at user log in or job execution.”



```
Daniel.Schornak@fe1:~  
[Daniel.Schornak@fe1 ~]$ module list  
No Modulefiles Currently Loaded.  
[Daniel.Schornak@fe1 ~]$
```

At Job Execution...



```
Daniel.Schornak@tfe1:~  
[Daniel.Schornak@tfe1 ~]$ module list  
No Modulefiles Currently Loaded.  
[Daniel.Schornak@tfe1 ~]$
```

Related Environmental Variables:

- MODULESHOME** - The location of the master Modules package file directory containing **module** command initialization scripts, the executable program **modulecmd**, and a directory containing a collection of master *modulefiles*.
- MODULEPATH** - The path that the **module** command searches when looking for *modulefiles*.
- LOADEDMODULES** - A colon separated list of all loaded *modulefiles*.
- _LMFILES_** - A colon separated list of the full pathname for all loaded *modulefiles*.

NESCC Factoid...

“At a minimum, you will want to:

- module load intel
 - module load mpt
- } module load intel mpt

Module Commands – “*module list*”

Sample Output
“*module list*”

```
[daniel.schornak@fe2 ~]$ module list
Currently Loaded Modulefiles:
 1) icc/11.1.072
 2) mvapich2/1.4.1-intel-11.1
 3) netcdf/3.6.3
 4) hdf4/4.2r3-intel
 5) hdf5/1.8.3
 6) ncl/5.2.0-intel
 7) intel/11.1.072
 8) papi/4.1.0
 9) nco/4.0.1
10) udunits/2.1.15
11) mathlibs/fftw
12) uberftp/2.7
13) gempak/5.11.4
14) jet-tools
15) sge
16) totalview/8.8.0-1
17) wjet
```

Sample Output
“*module -l list*”

```
jetrsa.rdhpcs.noaa.gov - PuTTY
[daniel.schornak@fe2 ~]$ module -l list
- Package -----+-- Versions +- Last mod. -----
Currently Loaded Modulefiles:
icc/11.1.072                2011/06/08 16:07:40
mvapich2/1.4.1-intel-11.1  2010/07/01 20:28:22
netcdf/3.6.3               2009/07/24 15:22:49
hdf4/4.2r3-intel          2010/08/12  2:21:30
hdf5/1.8.3                2010/05/30 14:59:42
ncl/5.2.0-intel           2011/07/12 22:16:56
intel/11.1.072            2011/07/12 23:16:03
papi/4.1.0                2010/06/25 20:28:44
nco/4.0.1                 2011/08/26 15:31:05
udunits/2.1.15            2010/07/09 22:37:56
mathlibs/fftw             2009/07/22 21:53:31
uberftp/2.7               2011/11/01 19:18:11
gempak/5.11.4             2011/02/07 17:46:01
jet-tools                 2011/11/01 19:17:39
sge                       2009/07/28 22:24:46
totalview/8.8.0-1        2010/05/25 16:08:12
wjet                      2010/07/09 22:34:55
[daniel.schornak@fe2 ~]$
[daniel.schornak@fe2 ~]$
```

Module Commands – “*module switch <this> <that>*” “*module swap <this> <that>*”

Change to a newer C compiler version (current: intel/intel-cc-12-12.0.4.191;
want: intel/intel-cc-12-12.1.0_sp1.6.233)

Before....

```
[Daniel.Schornak@tfe1 ~]$ module list
Currently Loaded modulefiles:
 1) intel/intel-cc-12-12.0.4.191      3) intel/intel-cmkl-12-12.0.4.191
 2) intel/intel-rc-12-12.0.4.191    4) intel/tools
```

Make the “Switch”...

```
module switch intel/intel-cc-12-12.0.4.191 intel/intel-cc-12-12.1.0_sp1.6.233
(same as: module swap intel/intel-cc-12-12.0.4.191 intel/intel-cc-12-12.1.0_sp1.6.233)
```

After...

```
[Daniel.Schornak@tfe1 ~]$ module list
Currently Loaded Modulefiles:
 1) intel/intel-cc-12-12.1.0_sp1.6.233
 2) intel/intel-rc-12-12.0.4.191
 3) intel/intel-cmkl-12-12.0.4.191
 4) intel/tools
[Daniel.Schornak@tfe1 ~]$
```

Module Commands – “*module show*”

Command shows what environmental variables are set and any associated modules

```
Daniel.Schornak@tfe1:~  
[Daniel.Schornak@tfe1 ~]$ module show intel  
-----  
/apps/modulefiles/intel/12-12.0.4.191:  
  
setenv      MPICC_CC icc  
setenv      MPICXX_CXX icpc  
setenv      MPIF90_F90 ifort  
module      load intelprod/cc/12-12.0.4.191  
module      load intelprod/fc/12-12.0.4.191  
module      load intelprod/cmkl/12-12.0.4.191  
-----  
[Daniel.Schornak@tfe1 ~]$
```

NESCC Factoid...

“Intel modules cannot coexist with PGI modules. Load one or the other, but not both!”

```
Daniel.Schornak@tfe1:~  
[Daniel.Schornak@tfe1 ~]$ module show pgi  
-----  
/apps/modulefiles/pgi/11.6:  
  
prepend-path MANPATH /apps/pgi/linux86-64/11.6/man  
prepend-path LM_LICENSE_FILE /apps/pgi/license.dat  
prepend-path PATH /apps/pgi/linux86-64/11.6/bin  
setenv      MPICC_CC pgcc  
setenv      MPICXX_CXX pgCC  
setenv      MPIF90_F90 pgf90  
-----  
[Daniel.Schornak@tfe1 ~]$
```

Module Commands – *What to watch out for!*

Version incompatibilities among modules can occur

Solution:

1. Remove all installed modules and build from scratch (*module clear*)
Note: “clear” is interactive; “purge” in non-interactive – same results

```
Daniel.Schornak@tfe1:~  
[Daniel.Schornak@tfe1 ~]$ module clear  
  
Are you sure you want to clear all loaded modules!? [n] y  
[Daniel.Schornak@tfe1 ~]$ module list  
No Modulefiles Currently Loaded.  
[Daniel.Schornak@tfe1 ~]$
```

2. Load only the modules that you require *

```
Daniel.Schornak@tfe1:~  
[Daniel.Schornak@tfe1 ~]$ module load intel  
[Daniel.Schornak@tfe1 ~]$ module list  
Currently Loaded Modulefiles:  
  1) intelprod/cc/12-12.0.4.191      3) intelprod/cmkl/12-12.0.4.191  
  2) intelprod/fc/12-12.0.4.191    4) intel/12-12.0.4.191  
[Daniel.Schornak@tfe1 ~]$
```

- *Note: Interdependent/compatible modules will automatically load*

3. Logging out and back in will provide a new session with no modules loaded

Introduction to Programming Environment

Recommended Exercises



1. Module appreciation exercise...
 - a. Unload all modules (*"module clear"*)
 - b. Verify Intel C compilers not available (*"icc -v; if77 -v"*)
 - c. Load and verify Intel compiler modules (*"icc -v; if77 -v"*)
 - d. *Load and verify PGI compilers (*"pgcc --version; pgf77 -version"*)

2. Modules for libraries
 - *Check library paths*

3. Ensure modules are loaded at login
 - Edit .profile file and add appropriate "module load" entries

4. Ensure modules are loaded at job execution
 - Include "module load <modulename>" in batch script

* Remember to *"module clear"* or *"module unload intel"* before loading *pgi*

Introduction to Programming Environment

NESCC Software Stack

Operating System	bbcp	gcc	GrADS	libtool	netCDF v4	Python netcdf module
Batch System	bbFTP	gdb	GRIB libraries and utilities	libxml	OpenMP	Python-numpy module
Batch System	Bison	Ghostview	gzip	Linux/UNIX debugger	Optimized BLAS	R (statistical package)
System Monitoring and Accounting	C/C++	Globus Toolkit	HDF4	McIDAS	Optimized FFTW	Ruby
ANTLR	Environment Modules	GNU binutils	HDF5	MP Toolbox, MPI, MPI-21/0	Perl	SVN/CVS
autoconf	ESMF	GNU coreutils	Heirloom cpio	NCAR Graphics	PETSc	Udunits v1.X
automake	FORTRAN 77/90/95	GNU make	ImageMagick	Ncview	Python	UNPACK
bash	gawk	GNU tar	Java	netCDF Operators	Python scipy module	X-11

Introduction to Programming Environment

Preparing for Job Submission – Batch Script Considerations

Use msub. Here is an example batch script:

```
#!/bin/sh --login
# -- Request 12 cores
#PBS -l procs=12
# -- Specify a maximum wallclock of 4
#PBS -l walltime=4:00:00
# -- Specify under which account a job
#PBS -A hpl
# -- Set the name of the job, or moab w
#PBS -N HPL
# change directory to the working dire
# Use the if clause so that this script stays portable
# if [ x$PBS_O_WORKDIR != x ];
then
cd $PBS_O_WORKDIR
fi
np=$PBS_NP
module load intel
module load mpt
mpixexec_mpt -np $np ./xhpl
```

NESCC Factoid...

In order to load module, make sure to use "--login" when declaring the script's shell...such as:

```
#!/bin/bash --login
#!/bin/ksh --login
#!/bin/sh --login
```

All jobs must declare their account identifier

```
#PBS -A <Project Name>
```

Introduction to Programming Environment

Finding your Account Information – *New Tool!*

Use: *account_params*

```
Daniel.Schornak@fe4:~  
[Daniel.Schornak@fe4 ~]$ account_params  
Account Params -- Information regarding project associations  
  
Processing Unix group file /etc/group  
User: Daniel.Schornak  
Project: nesccmgnt  
Allocation: Id Name Amount Reserved Balance CreditLimit Available  
Allocation: -- -----  
Allocation: 84 nesccmgnt 709127157 0 709127157 0 709127157  
  
Directory: /scratch1/portfolios/BMC/nesccmgnt DiskInUse=84173 GB, Quota=211500 GB  
Directory: /scratch2/portfolios/BMC/nesccmgnt DiskInUse=140185 GB, Quota=211500 GB  
  
[Daniel.Schornak@fe4 ~]#
```

NESSC Factoid...

account_params shows...

- *Project Name*
- *Project Allocation Balances*
- *Shows assigned Scratch Space Locations and Quotas*

Introduction to Programming Environment

Preparing for Job Submission – Batch Script Considerations (continued)

If you need to change the processor layout, there is a way. Use the nodes option.

#PBS -l nodes=4:ppn=6

Each node has 12 cores. The above syntax will allocate 4 nodes, and schedule 6 tasks per node. This is what you would want to do for an OpenMP job where each MPI process uses 2 threads.

Other examples:

#PBS -l nodes=12:ppn=1

Start job on 12 nodes, with one thread per node (For 12 MPI tasks, OMP_NUM_THREADS=12)

#PBS -l nodes=2:ppn=1+4:ppn=12

Start job with one process on each of the first two nodes, then fill up the last 4 nodes with 48 tasks - This would be for a job that has I/O tasks for the first two MPI ranks.

Introduction to Programming Environment

Optimizing performance for MPI applications using MPT

The default buffer settings used by the MPT MPI library are inadequate to provide decent performance for most applications. It is recommend that you set the following variables prior to calling `mpiexec_mpt`.

```
setenv MPI_BUFS_PER_PROC=128  
setenv MPI_BUFS_PER_HOST=128  
setenv MPI_GROUP_MAX=128
```

Hint: For more information: run “*man mpi*” after loading the mpt module

https://nescdocs.rdhpcs.noaa.gov/wiki/index.php/Using_MPI

Introduction to Programming Environment

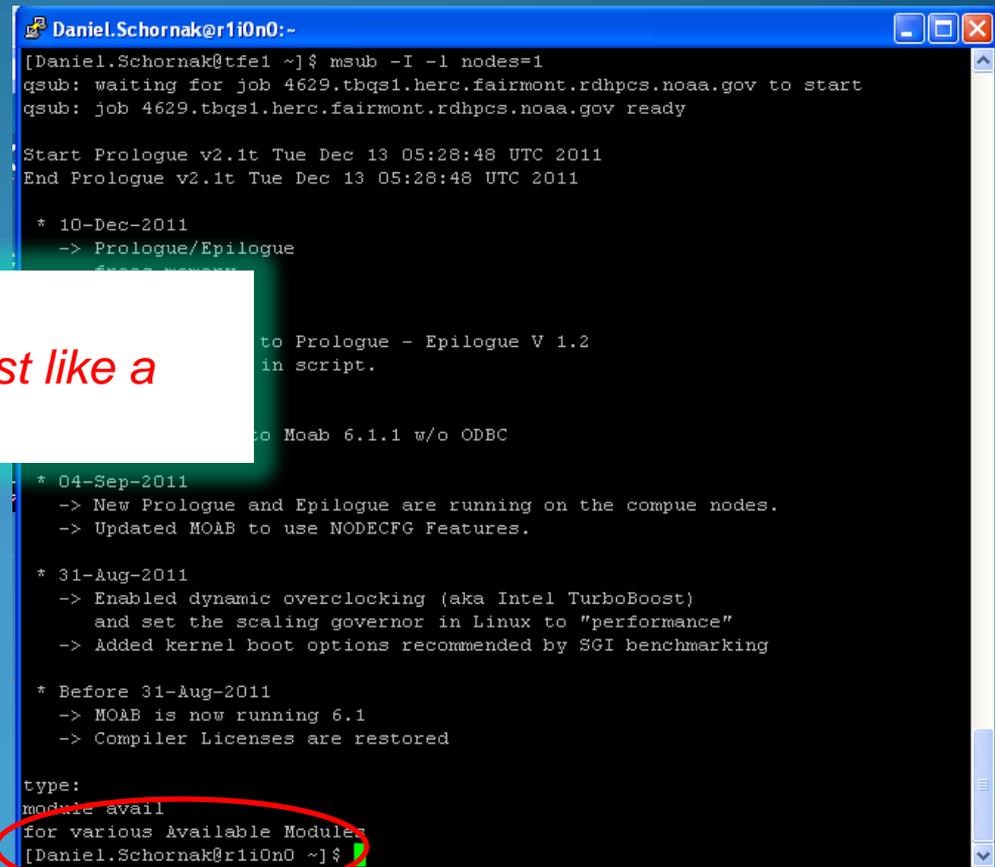
Interactive Job performance for MPI applications using MPT

If you need to do other interactive work, including running, development, or debugging of jobs, an interactive job is a great way to do this.
To create an interactive job, use the `-I` option to `msub`:

```
# msub -I -l nodes=1
```

NESCC Factoid...

“Interactive jobs can be any size – just like a normal batch job.”



```
Daniel.Schornak@r1i0n0:-  
[Daniel.Schornak@tfe1 ~]$ msub -I -l nodes=1  
qsub: waiting for job 4629.tbqsl.herc.fairmont.rdhpcs.noaa.gov to start  
qsub: job 4629.tbqsl.herc.fairmont.rdhpcs.noaa.gov ready  
  
Start Prologue v2.1t Tue Dec 13 05:28:48 UTC 2011  
End Prologue v2.1t Tue Dec 13 05:28:48 UTC 2011  
  
* 10-Dec-2011  
-> Prologue/Epilogue  
      f9000-xxxxxx  
  
      to Prologue - Epilogue V 1.2  
      in script.  
  
      to Moab 6.1.1 w/o ODBC  
  
* 04-Sep-2011  
-> New Prologue and Epilogue are running on the compue nodes.  
-> Updated MOAB to use NODECFG Features.  
  
* 31-Aug-2011  
-> Enabled dynamic overclocking (aka Intel TurboBoost)  
    and set the scaling governor in Linux to "performance"  
-> Added kernel boot options recommended by SGI benchmarking  
  
* Before 31-Aug-2011  
-> MOAB is now running 6.1  
-> Compiler Licenses are restored  
  
type:  
module avail  
for various Available Modules  
[Daniel.Schornak@r1i0n0 ~]$
```

Introduction to Programming Environment

Scheduler Commands Cross Reference Table

The table below reflects similar functions across the various schedulers within the NOAA HPC environments.

NCEP LoadLeveler Commands	ESRL SGE Commands	NESCC (and GFDL) Moab Commands	Function
llcancel	qdel	mjobctl -c	Cancels a submitted job
llclass	TBD	TBD	Returns information about job classes
llcc	TBD	TBD	Returns free cpus about job classes
llhold	qhold qrls	mjobctl -h mjobctl -u	Holds or releases a hold on a job
llq	sgestat qstat	checkjob showq	Queries the status of jobs
llstatus	qhost	showstate	Queries the status of machines
llsubmit	Qsub	msub	Submits a job
share_reporter.ksh	TBD	showstats	Reports the total share and used share for each group and user
TBD	userstat	qstat -Q	Displays node statistics and batch queue for cluster

Introduction to Programming Environment

Running an Openmp/MPI hybrid job

The previous instructions tell you how to request nodes and placement in a way to support OpenMP/MPI hybrid applications. However, it is necessary to include an additional command to get the processes of your job to be allocated correctly. To do this, use the *omplace* program. Example:

```
# mpiexec_mpt -np $NP omplace ./f.applic.x
```

By default, *omplace* will use the value set by `$OMP_NUM_THREADS`. If that value is not set, it will use 1. You can explicitly set the number of threads to be used by each MPI rank with the `-nt` option. Ex:

```
# mpiexec_mpt -np $NP omplace -nt 4 ./f.applic.x
```

In this example, each `f.applic.x` executable could use 4 threads. You still need to set `OMP_NUM_THREADS` to the correct value for your model run.

Online Documentation– Where to go...

Website

<https://nescdocs.rdhpcs.noaa.gov>

Access and Use of TDS

https://nescdocs.rdhpcs.noaa.gov/wiki/index.php/Access_and_Use_of_TDS

PGI Compilers User Guide

<http://www.pgroup.com/doc/pgiug.pdf>

Optimization with Intel Compilers

http://software.intel.com/sites/products/collateral/hpc/compilers/compiler_qrg12.pdf

NESCC Factoid...

“Documentation, such as listed above, will start to be made available on NesscDocs soon.”

Need Help? – *Where to go...*

Zeus User Support and Problem Reporting – Help Desk for NESCC
rdhpcs.zeus.help@noaa.gov

HPSS User Support and Problem Reporting – Help Desk for NESCC
rdhpcs.hpss.help@noaa.gov

NESCC Documentation Wiki Site – “How to...”
https://nescdocs.rdhpcs.noaa.gov/

End User Experience

EMC Model Transition Team (Provides updates for porting to TDS and Zeus)
http://www.emc.ncep.noaa.gov/mtt

NESCC Factoid...

“Additional documentation will continue to be made available on the NescDocs Wiki Site.”

Group A End User Training

- 0800-0810 Training Process
- Introduce instructors
 - General information
 - Define training roles and responsibilities
 - Review training agenda
- 0810-0815 Training Objectives
- Review the objectives of the NESCC HPC Environment overview
- 0815-0845 Introduction to NESCC HPC Design/Architecture and Environment
- Describe the overall architecture major components, functions, and features
- 0845-0900 Available On-line Documentation
- 0900-0915 **BREAK**
- 0915-0945 Introduction to User Environment, Policies, Quotas, and Environmental Variables
- 0945-1045 Introduction to Programming Environment
- Introduce tools – shells, applications, compilers, and libraries
- 1045-1145 Introduction to NESCC Storage and Data Management
- 1145-1245 LUNCH BREAK**
- 1245-1415 Introduction to Job Scheduling using Moab (Adaptive Computing)
- Efficient job submission techniques
 - Installed NESCC version compared to other NOAA installations
 - Moab/Torque end-user commands and tools
- 1415-1500 Questions/Answers
- 1500 Session Wrap up

Introduction to Job Scheduling using Moab (Adaptive Computing)

Shawn Hoopes – Adaptive Computing

Group A End User Training

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Group A End User Training – Wrap Up

Reminder: Please complete and return the Post-training Questionnaire

Additional Questions?

Dan Schornak: dschorna@csc.com

Need Help? – *Where to go...*

Help Desk for NESCC

rdhpcs.zeus.help@noaa.gov

HPSS Help Desk for NESCC

rdhpcs.hpss.help@noaa.gov

NESCC FAQ and Documentation Website

https://nescdocs.rdhpcs.noaa.gov/wiki/index.php/Main_Page

EMC Model Transition Team – Providing updates for porting to TDS and Zeus

<http://www.emc.ncep.noaa.gov/mtt>